Can the Paris Agreement stop global warming?

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Sustain ATV Conference 2016
Creating Technology for a Sustainable Society

DTU

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Table of Contents

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Sustainability

"Sustainable development seeks to meet the needs and aspirations of the present without compromising the ability to meet those of the future" [1]

A sustainable society is considered to involve a balanced interplay of three main elements to meet the needs of present generations without compromising the possibilities of future generations to meet their own needs [1]:

- The environmental boundary conditions that set the limits on resource supply, waste disposal and environmental pollution;
- How the economy balances production and consumption processes within – or currently beyond - the environmental constraints;
- How society politically and culturally decides to manage the social effects of the above constraints given by the short and long term consequences of our activities.

Our developing knowledge of our own environmental impact imposes limits on our activities, while our expectations to the quality of life we wish to have requires expansion of activities.

Radically improved efficiency of our technologies are urgently needed in order to reduce both reliance on scarce resources and the long term effects on the environment and the climate, but also to handle the longer term demographic changes and the increase in material wealth in developing economies.

Society's growing awareness of the many challenges is causing a gradual but unavoidable change in our perspective on technology, from the traditional optimization of economic cost with the specific technological performance to a much broader view including environmental impact and performance in terms of resource efficiency etc.These considerations are becoming increasingly important in how we direct R&D and assess emerging technologies.

Both citizens expectations and policies are evolving with this changing perspective. In 2015 UN formulated 17 Sustainable Development Goals that aims at making a series of important changes to create a more sustainable world over the next 15 year.

The many challenges are also targeted with research: The EU Commission states that "Sustainable development will be an overarching objective of Horizon 2020" and allocates 60% of the budget to this [2]. The Danish Forsk2020 has also made the technical challenges in creating a sustainable society an important factor in their scope.

Sustainability is hence becoming a core consideration for research and development, both in terms of finding technological solutions to the increasing number of societal challenges, but also as a fundamental requirement to any technology being developed for it to have a place in the future market of a sustainable society.

The Sustain Conference at DTU started out in 2014 as a conference where everyone involved in research at DTU from PhD students to Professors could meet to share their knowledge and inspire each other to create the best possible teams and solutions for solving the challenges.

The conference is now actively opening to invite researchers and industry to create a yearly recurring forum for sustainable technology in Denmark, and facilitate formation of collaborations between academia and industry.

The conference is divided into several parallel sessions, and these broadly speaking cover the main societal challenges on sustainability with regards to technology and the main technology domains at the host DTU and in Denmark.

[1] United Nations General Assembly (1987) Report of the World Commission on Environment and Development: Our Common Future. http://www.un-documents.net/our-common-future.pdf

[2] "Horizon 2020 - The Framework Programme for Research and Innovation" Communication from the Commission to the European Parliament, the Council, the European Economic and Social Committee and the Committee of the Regions 30.11.2011.

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Claus Stig Pedersen,
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Concluding comments by Henrik Kærgaard, Niras

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Session

A

Oral Presentations

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Range of technology choices in life cycle assessment of environmental treatment technologies: An example of a solid waste landfill model

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Limited data availability and local differences of environmental treatment technologies lead to the use of sub-optimal data and choices of single datasets, where multiple data choices may be representative. The use of data not representing the entire coverage of an LCA study can cause a bias in the result interpretation and limit the robustness of the results. The objective of this study is to demonstrate the relationship between the number of discrete data options and the goal and scope of the study. The importance of the spread in LCA results and how this spread influences the LCA result interpretation is assessed. The objective is obtained by performing a landfill model case study and presenting and discussing results relative to the specificity of the coverage of the study (see conceptual approach in Figure 1).

The outcomes shows a trend of decreasing LCA result ranges with increasing level of specification of the technological and geographical coverage of the study. For example, for global warming potential, the global maximum value is 2.6 times larger than the global minimum value and, for human toxicity, carcinogenic, the global maximum value is 45 times larger than the global minimum value. These ranges have the potential to significantly influence the LCA results, and are interpreted as potential magnitudes of errors introduced by the data choices. The results highlighted the pitfalls of choosing specific data to represent a generic process, and vice-versa. The former will lead to precise, but inaccurate results, whereas in the latter the obtained data represent a lower level of knowledge than the initial goal and scope.

To conclude, a detailed description of the coverage of the study and understanding of the technologies are necessary for representative life cycle inventory modelling. This conclusions was described in a step-wise approach for representative data choices and modelling. The outcomes shed light on the potential spread caused by discrete data choices in the modelling of environmental treatment technologies.

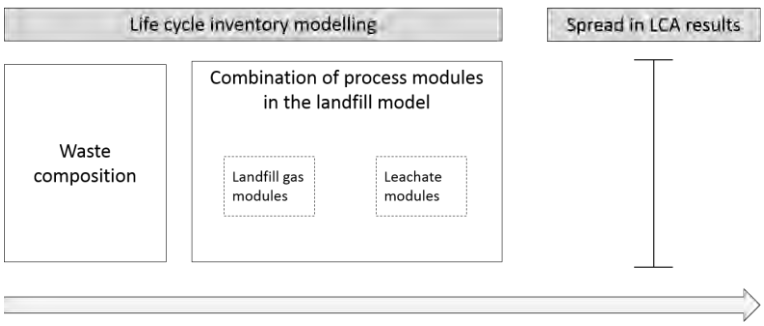

Figure 1: Conceptual approach of this study. Arrow indicates the order of activities.

Activity-based Sustainability Assessment of Highly Automated Manufacturing

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Sustainability of technology is a multifaceted endeavor and a main requirement from industry is to make it a profitable business case with clearly defined targets. To achieve that, a new assessment framework and applicable method [1] is presented which has been developed closely with industry. It uses a top-down decision-making process known from financial target setting for each cost center and the well-known life-cycle perspective according to ISO 14040 [2] in Sustainability Assessment. Thereby it is possible to allocate absolute environmental thresholds of functionalities (e.g. “transportation”) down to smallest production units by using activity-based target setting in a consistent way to lowers risks in the planning phase of products and production.

Success factors (SF), specifications and parameters are describing the manufacturability and therefore the revenue potential of products. By combining those with production and technology data, like cycle time, energy efficiency and material consumption as well as with expert opinion it is possible to determine an allocation method that predicts the so-called life-cycle targets (lct) for each cost center in manufacturing. A linkage to life cycle databases is established as well in order to predict environmental impact of the activities holistically (even divided into process, infrastructure and overhead). This approach allows to identify hotspots and can avoid sub-optimization within the different production levels as well as between different environmental impact categories.

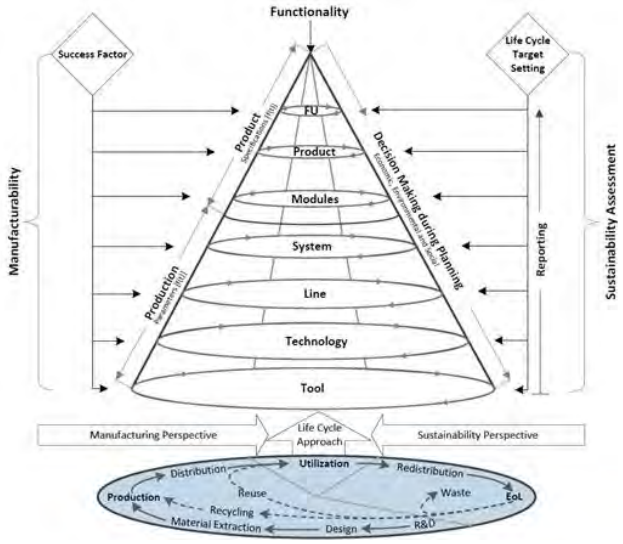

Figure 1 Sustainability Cone: Conceptual framework of merging life cycle perspective, product and production to derive life cycle targets (lct) thus optimizing product and production in an early planning phase [1]

This framework has been applied to a product life cycle of a standard passenger car, with emphasis on highly automated manufacturing. Lct’s for production cells and widely used technologies in highly automated car manufacturing will be presented followed by a discussion of how to use them in the decision making internally and externally in reporting schemes

[1] J.-M. Rödger, N. Bey, and L. Alting, “The Sustainability Cone – A holistic framework to integrate sustainability thinking into manufacturing,” *CIRP Ann. - Manuf. Technol.*, vol. submitted, 2016.
[2] ISO 14040, “Environmental management - Life Cycle assessment - Principles and framework,” Geneva, 2006.

On the need for integrating LCA into decision making

Yan Dong[1,2]*, Simona Miraglia[1, 3], Stefano Manzo[1,2], Stylianos Georgiadis[1,4], Hjalte Jomo Danielsen Sørup[1,5], Elena Boriani[1,6], Sebastian Thöns[1,3], Michael Z Hauschild[1,2]

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The need for sustainable solutions has gained attention both in academia and industry research due to increasing demands of human beings, which are incompatible with limitations in resources availability. Several methods, such as Life Cycle Assessment (LCA), were developed in the past decades to assess the environmental profile of products and services. However, when decision makers have several alternatives at hand to solve a problem, environmental performance is not the only criterion for choosing the best alternative. Other criteria such as risks and economical costs and benefits that are associated with the alternatives will also influence the final choice. Sometimes the most environmentally sustainable alternative may not be the safest or cheapest one. How to make a balanced decision considering environmental performance together with other criteria is not straight forward.

Decision analysis is broadly used to help decision makers identify the best solution among alternatives. The decision is based on expected utility generation, which incorporates consequences (or impacts) associated with each alternative. Depending on the research field and goal of the study, the included consequences can be e.g. environmental impacts, property damages from natural hazards and/or human health impacts. We examined the current decision analysis practice as it is applied in different research fields. The review shows that generally environmental impacts are considered less often than the other consequences. Meanwhile, LCA has been applied in many research fields to assess a wide range of environmental impacts associated with products or services. There is a huge potential for integrating LCA into other decisions analysis tools to include assessments of the environmental profile of alternatives. This will provide the possibility of systematical inclusion of environmental considerations in the decision making process, thus facilitating a more holistic decision. However, due to different scopes and purposes of LCA and other decision analysis tools, the integration is not straightforward. The lack of consistency in e.g. system boundaries and handling of uncertainty needs to be carefully managed.

Advancing absolute sustainability assessments of products with a new Planetary Boundaries based life-cycle impact assessment methodology

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The Planetary Boundaries (PB)-framework introduced quantitative boundaries for a set of biophysical Earth System processes. The PBs delimit a 'safe operating space' for humanity to act within to keep Earth in a Holocene-like state (Rockström *et al* 2009). The concept has gained strong interest from companies that want to assess and communicate the environmental sustainability of their products relative to the PBs. However, consistent methods for assessing environmental impacts of products and systems based on the PBs have, to date, not been developed (Ryberg *et al* 2016).

In this study, we developed an operational life-cycle impact assessment (LCIA) methodology where the definition of the impact categories is based on the control variables as defined in the PB-framework by Steffen *et al* (2015). This included the development and calculation of characterization factors for the Earth System processes considered in the PB-framework. The characterization factors cover environmental flows contributing to impacts on the Earth System processes (e.g. CO_2 and its precursors contributing to ocean acidification) and are expressed in the units of the PB framework's control variables (e.g. change in the aragonite saturation state per unit CO_2 emission for ocean acidification). The use of these characterization factors for evaluating the environmental impacts of products in LCA ensures impact scores that are compatible with the PB framework. The impact scores can be related to either the full PBs or an allocated safe operating space. The latter reflect the share of the safe operating space the assessed products can be considered entitled to, thereby, allowing for quantifying the absolute environmental sustainability of the products.

This new Planetary Boundaries based LCIA methodology provides additional and complementary insights which cannot be achieved with traditional LCIA-methodologies. The key added value is the ability to relate the impacts of a product to the Planetary Boundaries. This can be used for communicating a product's environmental performance and for setting reduction targets based on absolute environmental boundaries, thereby, advancing absolute sustainability assessments.

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Ryberg M W, Owsianiak M, Richardson K and Hauschild M Z 2016 Challenges in implementing a Planetary Boundaries based Life-Cycle Impact Assessment Methodology *J. Clean. Prod.* **139** 450–9

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Getting the chemicals right: addressing inorganics in sustainability assessments of technologies

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A main goal of sustainability research is to enable a technological development in industry and elsewhere that ensures that what is produced and how it is produced today does not harm the quality of human or environmental health for present and future generations. As part of current environmental sustainability assessments, the toxicity potential of several thousand organic chemicals is included in characterization models within life cycle impact assessment (LCIA). However, many economic production processes involve the use of inorganic chemicals to a large extent, while the related pressure on human and environmental health of environmental emissions of these substances is not yet fully understood and not included in any existing LCIA method. In this presentation, we provide an overview of the relevance of inorganic chemicals and outline possible ways towards incorporating inorganic chemicals in LCIA toxicity characterization.

Substances such as sodium sulfate decahydrate, sodium hydroxide, sodium carbonate, titanium(IV)oxide, and sodium hydrosulfite are used in large quantities e.g. in the textile industry [1], in the personal care sector [2] and/or in the building and construction industry. However, these inorganic substances are considered neither in current life cycle inventory databases nor in state-of-the-art LCIA characterization models. While some specific inorganic substances are included in impact assessment models for climate change (e.g. sulphur hexafluoride or carbon dioxide) or eutrophication (e.g. phosphorus pentoxide or nitrogen dioxide), human and eco-toxicity assessment models do currently not consider any inorganic substances except some cationic metals. Without the integration of inorganic substances such as salts, acids, bases and elements, however, no conclusions regarding the environmental sustainability of any technology containing any of these substances can be drawn.

The modelling approaches for different substance groups will be contrasted, for which a simple approach based on Kow is not suitable to characterize toxicity-related impacts, such as cationic metals, nanoparticles, and perfluorinated alkylated substances (PFAS). Differences in physicochemical properties and environmental fate of these specific substance groups compared to inorganic substance groups like acids, bases, and salts will be discussed. Furthermore, an approach to address environmental impacts like increased salinity as well as possible relevant chemical reaction pathways as a first step towards an adapted fate modelling toward a broader set of inorganic substances will be outlined as a necessary step toward improving the assessment of environmental sustainability of technologies containing inorganic substances in their life cycle.

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[2] National Library of Medicine. Household Products Database. Last modified: September, 2016. Available from URL: http://householdproducts.nlm.nih.gov/index.htm. Accessed on November 10, 2016.

Session

A

Laptop Presentations

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Nordic organizational style and how it may support design for sustainability implementation

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Design for sustainability (DfS) implementation in companies has been discussed and studied in academic literature from different perspectives, both technical and human related aspects included. The latter focus in literature has stressed upon the need for focus on the organizational characteristics, functioning style, communication patterns etc. as important determinants in DfS implementation in companies. It is in this context that this research work tends to explore if regional characteristics, that can be observed in companies, contribute/impact to the successful implementation of DfS in companies. As a case of reference, the Nordic their organizational style and its aptness presented in literature is studied and presented.

The Nordic industries have been one of the first movers on sustainability-related topics. This research work aims at exploring the Nordic style in organisations in a DfS context and is based on findings from existing literature and industrial reports in a broader field of research pertaining to the Nordics. The work investigates and presents factors and drivers that distinguish the Nordic countries from the rest of the world. A preliminary framework is also presented as part of the work to highlight how some of the most discussed DfS implementation challenges may be mitigated by the Nordic organizational style. Such an understanding may in turn inform a discussion on the potential need for customised tools, methods and approaches for implementing DfS within Nordic industry and beyond.

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Session

A

Poster Presentations

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How to consistently make your product, technology or system more environmentally-sustainable?

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Human activities are currently unsustainable, causing many damages to ecosystems, human health and natural resources. In this setting, the development of new products and technologies has been increasingly required to relate to sustainability and ensure that such development goes hand-in-hand with low environmental impacts, low-carbon emissions, low environmental footprints or more sustainability as a whole. To enable a scientifically-sound and consistent documentation of such sustainable development, quantitative assessments of all environmental impacts are needed. Life cycle assessment (LCA) is recognized as the most holistic tool to address that need. LCA has two main strengths: (1) the ability to quantify all relevant environmental impacts – not just climate change, but also metal depletion, water use, toxicity exerted by pollutants on ecosystems and human health, etc.; and (2) making the assessment of the product/technology in a life cycle perspective, from the extraction of raw materials through production and use/operation of the product up to its final disposal. Fully embracing these 2 features enables to minimize the risk of burden-shifting, e.g. if impacts on climate change are being reduced while increasing other relevant environmental impacts or if impacts are shifted from the use stage of a product to the manufacturing stage as a result of a change in the product composition. Here, we provide a glimpse at how LCA can help for eco-design purposes, moving towards the use of low-impact materials, identifying environmental hotspots (parts of the life cycle with largest environmental impacts), making prospective simulations through scenario analyses, comparing and selecting most environmentally-friendly product/technology alternatives, reporting on the environmental performances of the system. We rely on state-of-the-art science in the food sector, the aquaculture sector and the energy sector to showcase and illustrate the potential of LCA to undertake the environmental sustainability challenge and support product/technology/system development.

How to evaluate the environmental performance of Product/Service-Systems (PSS)?

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Popular concepts such as “circular economy”, “sharing economy”, and “service economy”, often promote that more sustainable businesses can be created when offering product performance (e.g. lighting as a service) rather than selling products (e.g. light bulbs). These types of offerings are often termed Product/Service-Systems (PSS). However, offering or buying a PSS does not necessarily lead to environmental improvements, as highlighted by several examples (such as car sharing). Due to a set of challenges with the current methodologies, the actual environmental performance of PSS is traditionally rarely quantified. The guidelines developed in this research (Figure 1) are intended to support studies that aim to explore if or when a PSS is leading to environmental improvements.

The guidelines are built on Life Cycle Assessment (LCA) and can be applied at different stages and by different users, e.g. designers and decision-makers. They aim at guiding the user to perform a study, where the environmental performance of a PSS is objectively evaluated and quantified; taking a holistic perspective when comparing different options for needs fulfilment. Focus is on analysing the environmental impact changes when a PSS is compared to a reference system.

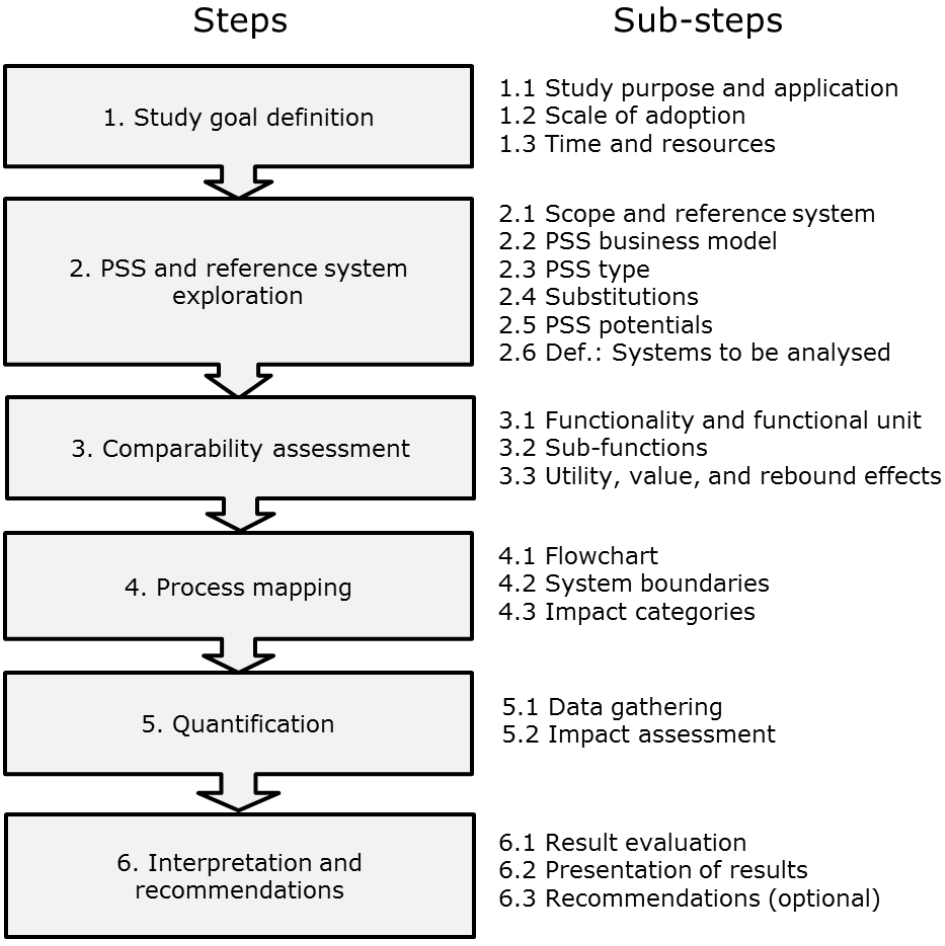

Figure 1: Guideline steps and sub-steps for PSS environmental evaluation

Inter-organizational cooperation for greener products and services

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The business world experiences an increasing attention to sustainability topics. In response to their stakeholders' concerns or following their own aspirations, more and more companies develop their approaches to sustainability. Life-cycle thinking recommends companies to integrate their sustainability strategies into a value chain perspective in order to avoid burden shifts from one life-cycle stage to another. Certain decisions impacting products' and services' life-cycle may be taken at a given company, while others are likely to be beyond the direct control of the company and require to be managed through inter-organizational interactions. Numerous scholars call for increased cooperation between companies on green issues. On the other hand, the business world experiences a current development in sustainability approaches deeply rooted in inter-organizational cooperation such as circular business strategies, green supply chain initiatives, and target setting on a value chain level. Current literature on green management reveals that cooperation practices across companies on green issues are still rare, that implementing cooperation practices is challenging and that there is a need for shift in focus from why companies should develop sustainability strategies to how they may implement the latter. In our on-going study, we base our approach on the contingency theory and build on inputs from academia to develop a conceptual management model aimed at supporting the discussion and reflection for a given company about its current or possible cooperation practices with other companies, in a context of greener products or services. Moreover, this model is elaborated to support identifying the existence of companies' archetypes towards inter-organizational cooperation. The up-to-date model is elaborated around three main areas: factors influencing cooperation practices, cooperation approaches and cooperation activities.

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Towards circular economy strategies from a company perspective: How should sustainable "closed-loops" look like for a given product?

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In the global strive towards more sustainable solutions, Circular Economy is seen as a central approach since it aims at a.o.t. closing material loops and thus at reducing the necessity to extract (new) raw materials for new products. While this overall idea is easy to understand, it is not easy to identify from a company perspective, what types of closed loops would be preferable – ranging from completely open loops to fully closed loops entirely under control of the company – and which implications the different options yield in terms of economic viability, technical feasibility and environmental sustainability. Also, the number of company-external stakeholders to involve in each alternative differs, depending on the type of loop and, not the least, depending on the type of product and concrete markets, the product shall be sold on. At the same time, systematic support in finding suitable pathways towards closed-loop solutions does not exist.

This project aims at developing the foundations for such support; namely a systematic and integrated approach to identify candidate pathways. Key idea is to, firstly, combine state-of-the-art insights from the knowledge pools "Technology", "Business models", and "Sustainability assessment" in an integrated closed-loop system approach (fig. 1), and, secondly, to apply it to assess selected scenarios against the target factors "Climate impact/Abatement potential" and "Economic impact & viability".

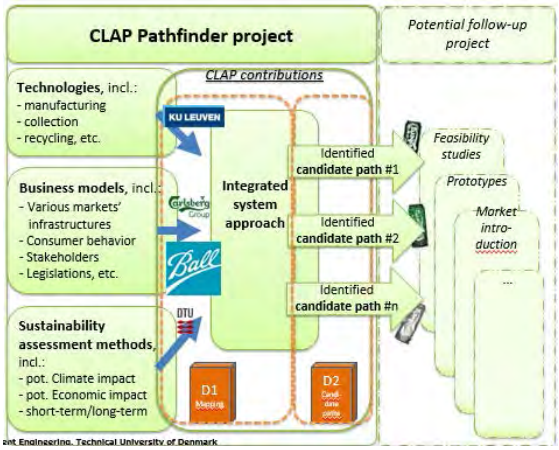

Figure 1 *Illustration of elements, project flow and targeted outcomes of the CLAP project.*

Chosen product context is that of aluminium beverage cans and the approach is being developed with partners covering four key areas of recycled can systems: Carlsberg A/S, expressing the B2C demand, Ball Corp., being a B2B supplier, and two leading universities in recycling technology and sustainability assessment, incl. sustainable business models – KU Leuven and DTU.

Expected results are 1) A comprehensive mapping of state-of-the-art knowledge in three key knowledge pools that currently are rather separated (i.e. aluminium recycling technologies, circular business models, and sustainability assessment methods) 2) Two-three identified high-potential candidate paths that qualify for feasibility testing in an intended follow-up project, wrt. technology and conditions on different markets globally (economy, infrastructure, consumer behaviour, etc.). Expected CO2e-impact reduction from the combined infrastructure/technology approach is at least 10-15% compared to today.

The project Closed-Loop Aluminium Post-consumer waste recycling (CLAP) receives funding from the Climate-KIC Nordic program.

Session

B

Oral Presentations

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Combining metabolic engineering and biocompatible chemistry for efficient production of food ingredients

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Abstract

Biocompatible chemistry, that is non-enzymatic chemical reactions compatible with living organisms, is gaining increasing attention because of its potential within biotechnology for expanding the repertoire of biological transformations carried out by enzymes. Here we demonstrate how biocompatible chemistry can be used for synthesizing valuable food ingredients as well as for linking metabolic pathways to achieve redox balance and rescued growth. By comprehensive rerouting of metabolism, activation of respiration, and finally metal ion catalysis, we successfully managed to convert the homolactic bacterium *Lactococcus lactis* into a homo-diacetyl producer with high titer (95 mM or 8.2 g/L) and high yield (87% of the theoretical maximum). Subsequently, the pathway was extended to (*S*,*S*)-2,3-butanediol (S-BDO) through efficiently linking two metabolic pathways via chemical catalysis. This resulted in efficient homo-S-BDO production with a titer of 74 mM (6.7 g/L) S-BDO and a yield of 82%. The diacetyl and S-BDO production rates and yields obtained are the highest ever reported, demonstrating the promising combination of metabolic engineering and biocompatible chemistry as well as the great potential of *L. lactis* as a new production platform.

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Session

B

Laptop Presentations

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Session

B

Poster Presentations

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Development of metabolite profiling and metabolomics tools for *Pseudomonas taiwanensis VLB120*

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2: Co-supervisor, DTU Biosustain, Technical University of Denmark (DTU)
3: Main supervisor, DTU Biosustain, Technical University of Denmark (DTU)

Pseudomonas sp. VLB120 is a biofilm-forming Gram negative aerobic strain that isolated from soil at *Institute of Microbiology*, University of Stuttgart, Germany. The strain has an ability to survive and even able to grow in the presence of toxic solvents including octanol, toluene, and styrene. Furthermore, this strain utilizes a wide range of substrates including xylose which is the main component of hemicellulose that accounts for approximately 25 percent to 40 percent of lignocellulose. Therefore, it's clear that the strain is an idea for the production of different pharmaceuticals, chemicals or biofuels from renewable lignocellulosic biomass.

However, this strain might not produce naturally the practical outcomes desired by humankind; they might require gene modification or new metabolic pathways for production of valuable products. Since these approaches are metabolically demanding, absolute quantification of intracellular metabolites are critical to understand the metabolism of the cell, as concentrations impact both the free energies and rates of metabolic reactions. However, analysis of intracellular metabolites is a challenging task due to their fast turnover rate and chemical diversity. Therefore, methods used for quenching metabolism and extracting the metabolites to investigate the *in vivo* metabolic state of a cell at a given specific conditions are crucial in metabolomics studies, as they significantly affect the number and intensity of metabolites detected.

In this study we are investigating the metabolic state of P.VLB120 strain and testing the suitability of commonly used metabolomics tools for this strain, as many of the tools were designed for specific classes of metabolites or microorganisms.

Developing Lactic Acid Bacteria for the conversion of brown macroalgae into green chemicals and fuels

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Microbial conversion of biomass plays a major role in establishing a bio-based economy, which aims at replacing fossil resources with renewable substrates for the production of fuels and chemicals. Current efforts in using non-edible ('second generation') biomass rather than food-derived sugars focus on lignocellulosic materials such as crop residues and non-edible plants. However, lignin is often toxic to the production organism and hard to eliminate, and economically feasible conversion of cellulose and hemicellulose is still challenging. An attractive alternative includes brown macroalgae or sea weed, which do not contain lignin, do not require fresh water, are not a major food source, and contain a higher sugar fraction. The main sugars are mannitol, laminarin (glucose) and alginate (guluronate and mannuronate). We will use metabolic engineering and laboratory evolution of Lactic Acid Bacteria (LAB) for the conversion of brown macroalgae into green chemicals and fuels. To select the best-suited production platform, we are screening *Lactobacillus* and *Pediococcus* strains for traits like genetic accessibility, substrate utilization and several stress tolerances. Most microorganisms, including LAB, do not naturally utilize alginates and hence the introduction of these pathways will be the first step in engineering the selected strain, after which further efforts will focus on co-utilization of the different sugar fractions and establishment of product pathways.

Acetoin and 2,3 butanediol isomers synthesis in metabolically engineered *Lactococcus lactis*

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Harnessing the biosynthetic machinery of living cells is a common approach used for producing a broad range of useful chemicals. Here, we divert inherent metabolic routes in *L. lactis* to produce (3R)-acetoin and the derived 2,3-butanediol isomers. Efficient production of (3R)-acetoin was accomplished using a strain where the competing lactate, acetate and ethanol forming pathways had been blocked. By introducing different alcohol dehydrogenases into this strain, either EcBdh from *Enterobacter cloacae* or SadB from *Achromobacter xylosooxidans*, it was possible to achieve high-yield production of m-BDO or R-BDO respectively. To achieve biosustainable production of these chemicals from dairy waste, we transformed the above strains with the lactose plasmid pLP712. This enabled efficient production of (3R)-acetoin, m-BDO and R-BDO from processed whey waste, with titers of 27, 51, and 32.1g/L respectively. The corresponding yields obtained were 0.42, 0.47 and 0.40 g/g lactose, which is 82%, 89%, and 76% of maximum theoretical yield respectively. These results clearly demonstrate that *L. lactis* is an excellent choice as a cell factory for transforming lactose containing dairy waste into value added chemicals.

Increasing Oil Bodies in *Physcomitrella patens* by Overexpressing Oil Body-Associated Proteins

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In bryophytes, reproductive organs contain large amount of oil bodies (OBs), the well-known lipid-containing structures. OBs in spores are the most prominent and have been extensively studied. They are thought to be formed by budding off the outer layer of the endoplasmic reticulum membrane (ER) due to accumulation of neutral lipids between the leaflets of the phospholipid bilayer. In P. patens, the OBs are abundant in the mature sporophytes or during starvation, but are hardly observed in the vegetative stage. We overexpressed OB-associated proteins such as oleosin, seipin, and fibrillin to increase the OB formation in P. patens vegetative tissue. As a result, we confirmed that the number of OBs were significantly increased in the protonemal cells compared to the wild type. These structures could be used to compartmentalize, synthetically made high-value compounds in green cells.

Seamless gene editing in Aspergillus species, using CRISPR-Cas9

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Many fungi are both excellent degraders of biomass and natural producers of industrially interesting compounds, making them good candidates for cell factories. Several members of the genus Aspergillus are successfully used as industrial cell factories for production of organic acids, enzymes and other primary or secondary metabolites, and many other Aspergilli are currently being sequenced and might possess traits making them similar suitable as potential cell factories. Yields from such cell factories can be greatly enhanced by employing genetic engineering strategies, however there are several obstacles slowing down the process.

The harnessing of the prokaryotic and archaeal immune mechanism CRISPR (clustered regularly interspaced short palindromic repeats) as a tool for genetic engineering in eukaryotes, has proved to be a powerful technology. CRISPR/Cas9 introduces specific DNA double strand breaks (DSB) with high precision, which in turn can be employed to efficiently stimulate gene targeting. Consisting of two components, an RNA guided nuclease Cas9 and a chimeric guide RNA (gRNA), a specific DSB can be produced in the host organism, which can be utilized to facilitate precise gene editing. The cleavage target site is determined by 20 base pairs (bp) in the gRNA, and by exchanging those 20 bp, Cas9 can be programmed to target a specific chromosomal location with few constraints. The technology has had a huge impact on genetic engineering of organisms, such as plants or mammalian cells where gene targeting is notoriously inefficient, but has only recently been adapted to filamentous fungi.

When using conventional strategies for genetic engineering in filamentous fungi, most strategies results in a genetic selection marker being left behind at the site of the edit, which can affect metabolism and negatively impact downstream processing. Here we present methods allowing for seamlessly inserting or deleting genes, for precisely introducing point mutations without changing the surrounding sequence, and a simple assay to easily identify efficient gRNAs. Together these methods provide a valuable addition to the genetic toolbox of several species of industrial relevant *Aspergillus* species, which can greatly accelerate the development of new fungal cell factories.

Magnetosome production and functionalization

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Magnetotactic bacteria produce magnetic particles, which enable them to migrate along the magnetic field lines in the environment they live in. The magnetic particles called magnetosomes are nanometer sized lipid bilayer encased uniform crystals of magnetite (Fe_3O_4) or greigite (Fe_3S_4). Their magnetic properties make them potentially useful in many biomedical and technological applications, such as drug delivery, magnetic resonance imaging, immunoassay and magnetic markers. Making them an alternative to chemically synthesized magnetic nanoparticles. *Magnetospirillum gryphiswaldense MSR-1* as a model organism used to produce magnetosmes and is known to require a low dissolved oxygen (DO) concentration and iron during cultivation for magnetosome production. However, the relationship between these parameters and fermentation behavior is not well understood.

We will present a study where we investigate how the addition of iron impacts the physiology of the MSR-1 cells and the expression of key genes involved in the production of mangetosomes.

Furthermore, utilization of magnetosomes for applications as immunoassays requires the functionalization of the magnetsomes. Functionalization of the magnetosomes is achieved by attaching functional moieties to the magnetosome. We will present the work of functionalizing the magnetosomes for immunoassay by expressing IgG binding domains on the surface of magnetosomes.

Session

E

Oral Presentations

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The Villum Center for the Science of Sustainable Fuels and Chemicals

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The research of the VILLUM Center focuses on solving two of the major challenges in order to meet the political objective of achieving a fossil-free society by 2050. The transition from fossil fuels to renewable energy sources call for:

1. More efficient storage of renewable energy
2. Viable alternatives to chemicals, plastics and other materials which are currently produced by using oil and coal—as well as finding alternatives to fossil-based fuels for aircraft, for example, which cannot be electrified and thus exploit renewable energy.

The key to both challenges is to develop better catalysts to promote the various chemical processes. The center will develop a systematic methodology to accelerate the discovery process for new catalysts. It will do that in a concerted effort, which is composed of six interdependent sub-projects closely interlinked.

Denmark is the international leader within both catalyst research and production. The research center hopes to achieve a research breakthrough in the area, which in turn can pave the way for further technological development—ensuring that the exploitation of renewable energy in future will be so efficient that it can compete with fossil fuels and in the long term completely replace them.

Smart Energy Network's recommendations for research, development and demonstration of smart energy in Denmark

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Smart Energy Networks
Research, Development and Demonstration

The Danish 'Partnership Smart Energy Networks – Research, Development and Demonstration' has formulated 15 recommendations for research, development and demonstrations within smart energy, all supporting the national goal to become independent of fossil fuels by 2050. Several roadmap reports indicate that it is both technical possible and economic realistic to get there. The Partnership believes that smart integration of the energy system is core of the solution. However, the transition of the energy system takes time, there are many, possible solutions and ways to follow, and there are many strategic decisions to be taken on the way. The recommended immediate actions contribute to establishing a solid decision basis, ensuring that the necessary and best solutions will be available in due time.

The short form of the recommendations – divided in five themes – are:

- *Commercial technologies in new contexts*
  - [1] Extended system functions to existing commercial technologies
  - [2] Communication of system functions for existing commercial technologies
  - [3] Business models for providing system services
- *Extended integration of the energy sectors*
  - [4] Efficient and controllable conversion and storage technologies
  - [5] Data access across sectors and actors
  - [6] Large-scale energy lab for smart, integrated energy solutions
- *The right load at the right time*
  - [7] Energy flexible solutions within all fields
  - [8] Realising energy flexibility in real
  - [9] System solutions suitable for local energy generation
- *Planning and operation of smart energy systems*
  - [10] Optimised investments in energy infrastructures
  - [11] Methods for operation planning of integrated energy systems
  - [12] Stable operation of energy systems with fluctuating generation
- *Markets and business models for smart energy*
  - [13] Re-design of the future market based energy system
  - [14] Efficient market design for high wind and solar penetration
  - [15] Partnerships and roles supporting smart solutions

Local sustainable district energy cases from across Europe

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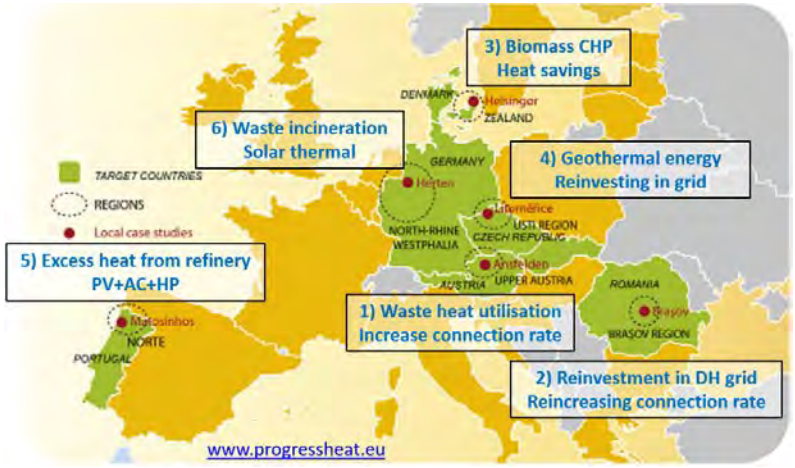
In the progRESsHEAT project, six local cases are analysed. The main objective of the progRESsHEAT project is to support policy makers and public authorities at local, regional and national level in the development and implementation of integrated strategies and policies to enforce the use of renewable and efficient heating and cooling solutions in their regions.



The main pillar of the strategy development process are local case studies for six municipalities. The goal of these case studies is to develop heating and cooling strategies through a profound analysis of (1) heating and cooling demands with respect to future developments, (2) long-term potentials of renewable energies and waste heat in the regions, (3) barriers & drivers and (4) a model based assessment of policy intervention in scenarios up to 2050 together with the authorities.

For this purpose we apply a geographic information system (GIS) and map the energy demands based on modelling of buildings and industry, the potential RE sources (including biomass, solar, geothermal, etc.) as well as waste heat sources and the existing energy production plants locally for each municipality. The district energy system of each municipality is then modelled in a coherent energy system analysis tool (EnergyPRO) which combines the detailed demand side modelling with the geographical overview of the resources and the existing production plants. The costs of providing district energy is then entered into a cost curve tool where the cheapest solution is found, depending on the location and type of building, comparing 1) district energy costs to 2) costs of increased energy efficiency and 3) costs of individual energy solutions. Thereby, the most cost effective solutions to increase RES heating and cooling at local level are identified.

Recent results from the local case studies will be presented, illustrating business cases for district heating in different regions in EU as well as the key success factors and main challenges and barriers for increased efficiency and sustainability of the European heating and cooling sector.

Physical model tests for floating wind turbines

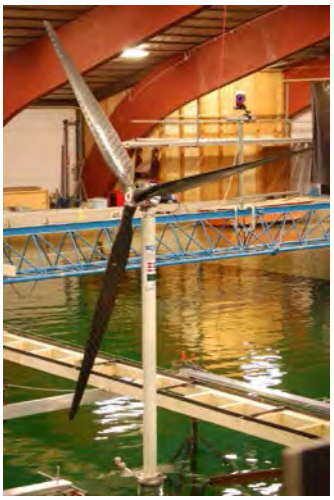
Henrik Bredmose*[1], Robert Mikkelsen[1], Michael Borg[1], Antonio Pegalajar-Jurado[1], Frank Lemmer[2]

1: DTU Wind Energy; 2: University of Stuttgart

Floating offshore wind turbines are relevant at sites where the depth is too large for the installation of a bottom fixed substructure. While 3200 bottom fixed offshore turbines has been installed in Europe (EWEA 2016), only a handful of floating wind turbines exist worldwide and it is still an open question which floater concept is the most economically feasible.

The design of the floaters for the floating turbines relies heavily on numerical modelling. While several coupled models exist, data sets for their validation are scarce. Validation, however, is important since the turbine behaviour is complex due to the combined actions of aero- and hydro-dynamic loads, mooring loads and blade pitch control.

The present talk outlines two recent test campaigns with a floating wind turbine in waves and wind. Two floater were tested, a compact TLP floater designed at DTU (Bredmose et al 2015, Pegalajar-Jurado et al 2016) and the recent Triple Spar design of Stuttgart University (Lemmer et al 2016). Both were built at a model scale of 1:60 along with a 1:60 scale version of the DTU 10MW reference wind turbine with a re-designed rotor, applicable to the low wind speeds of the lab. As a new development, the turbine was modified to enable active blade pitch control for the Triple Spar campaign.



The talk presents the scaling considerations and experimental design. The turbine was tested with rotor and floater ID tests and a range of wave conditions spanning from simple regular waves over focused wave groups to misaligned stochastic sea states. The floater and turbine response to combined wind and wave forcing are shown, with focus on aerodynamic damping from the wind and the effect of the controller. The results and analysis of these experiments for a new floater and with enabled pitch control contributes to a better understanding of the dynamics of floating wind turbines and improved validation of the numerical models.

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Session

E

Laptop Presentations

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Investigation of CO_2 reduction products on mass selected Cu nanoparticles

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The electrochemical reduction of carbon dioxide is a means of reversing the combustion of fuels. The process can be used to make various fuels and valuable chemicals in the form of hydrocarbons and oxygenated organics. The energy required for the electrolysis would come from renewable sources such as solar and wind and the CO_2 from point emission sources. In the 1980s Hori showed that a wide selection of reduced CO_2 products could be formed on polycrystalline Cu including methane and ethene[1,2]. Since then, various advances have been made in the field and particularly nanostructuring of Cu has been found to give high faradaic efficiencies at low overpotentials[3,4]. Particularly, high efficiencies for liquid fuel products such as methanol and ethanol are of interest.

Figure 1: Liquid cell for measurement of CO_2 reduction products. Shown here with a Cu sheet electrode as electrocatalyst.

The project will be measuring the product distribution from CO_2 reduction on samples of mass selected nanoparticles of Cu. The nanoparticles will be made using the SURFCAT cluster source. Both the size (mass) and the dispersion of the particles will be varied. The products will be measured with a combination of gas chromatography, head space-gas chromatography and NMR, similarly to previously reported in our department[5].

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Alternative NOx abatement, finding a suitable method

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Formation of NO_x during high temperature combustion with air is inevitable and of increasing environmental concern. NO_x participates in detrimental photochemical reactions in both the stratosphere and the troposphere, depleting the ozone layer and contributing to the greenhouse effect. Furthermore, higher NO_x concentrations cause severe health conditions, such as cancer and several respiratory diseases. The main constituent of NO_x in flue gas is nitric oxide (NO).

In larger installations, NO_x is removed by selective catalytic reduction (SCR) using a transition metal catalyst to facilitate reduction of NO_x with ammonia. SCR exhibits excellent conversions and selectivity, when run at temperatures around 300ºC.

In order to reduce their carbon footprint, several countries have begun experimenting with, and implementing, biomass firing in power plants. The catalytic activity of the traditional high dust SCR setup decreases significantly within the first few hundred operating hours, when firing biomass. The poisoning of the catalyst is mostly due to alkaline aerosols. The deactivation can be overcome by placing the SCR reactor at the tail end of the flue gas treatment system, the low dust position. At this point however, the temperature of the flue gas has decreased significantly and a costly heat exchange becomes necessary in order to remove the NOx via SCR. The deactivation is also a problem in the maritime industry, in waste incineration plants etc.

Due to the need for limiting CO_2 emissions, it is paramount that the current DeNOx portfolio is also expanded. So the need to remove one does not compromise the possibility of removing the other.

This project explores the possibility of removing NOx through one of several strategies utilising the unique properties of ionic liquids (ILs), including absorption and oxidation of NOx to nitric acid. The catalytic cycle for the latter reaction is shown in figure 1.

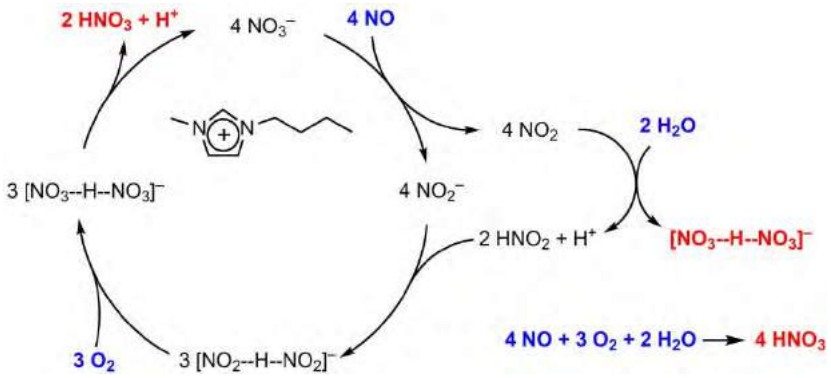

Figure 1: Catalytic cycle for the oxidation of NO in ionic liquids. In this case the 1-butyl-3-methylimidazolium cation is depicted, but research has shown other cations to also be active in this reaction.

Session

E

Poster Presentations

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A Web Based Approach to Model Efficiencies of Solar Fuels Devices

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While the sun irradiates earth with 120,000 TW, the world only consumes 17 TW, thus there is ample solar energy to power society. However one of the largest issues with solar power is its intermittency and inability to provide a concentrated energy source. By using a photovoltaic to produce molecular fuels rather than electricity, we can resolve both of these issues. However there are many parameters to be optimized in such a system to maximize efficiency. We will demonstrate how one can model these systems and analyze how varying any of the parameters affects performance.

We will take parameters using state of the art solar cells, catalysts, and electrolytes and use this to show what would be the optimal efficiency for reactions such as H_2 evolution, CO_2 to formate production, and CO_2 to CO production. Figure 1A is an example of modeling the efficiencies for water splitting reaction. We will also show a combined experimental and modeling approach to analyze state of the art devices to determine where we can make the greatest gains in efficiency (as shown in Figure 1B).

The entire model was created using a web based platform, and is located at www.SolarFuelsModeling.com for anybody to use.

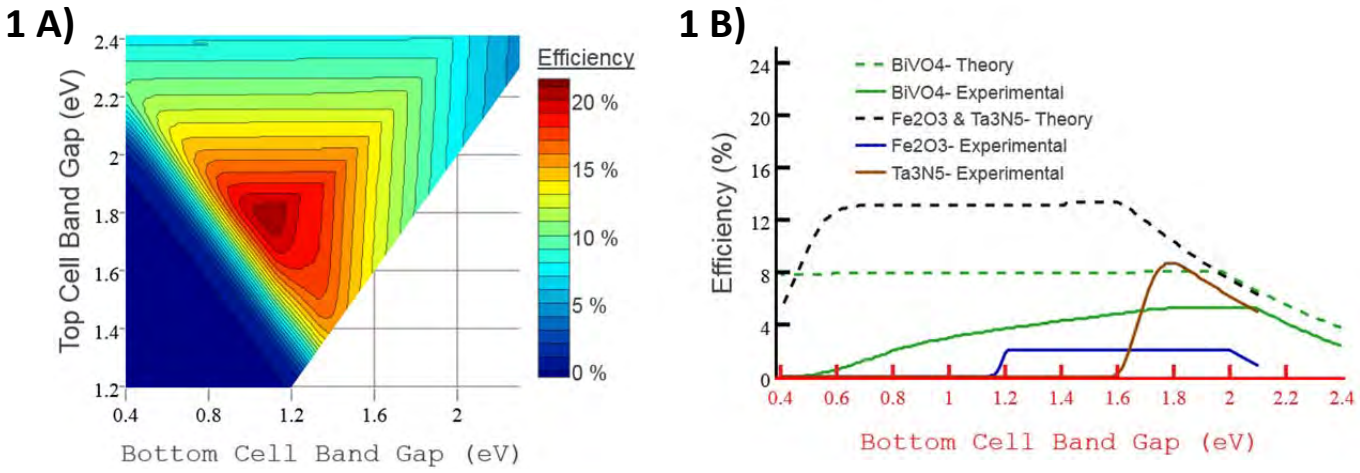

Figure 1: Efficiencies for H_2 evolution using 2-photoabsorbers tandem solar cell. A) Using purely theoretical results. B) Using data based off of one theoretical photoelectrode and either an experimental photoelectrode or another theoretical photoelectrode with the same band gap as the experimental photoelectrode.

Exploiting the energy source of the stars: Fusion energy research at DTU

J. Rasmussen*, T. Jensen, M. Jessen, S. B. Korsholm, A. W. Larsen, F. Leipold, J. Madsen, M. L. Magnussen, V. Naulin, A. H. Nielsen, S. K. Nielsen, J. M. B. Olsen, J. J. Rasmussen, M. Salewski, M. Stejner, A. S. Thrysøe

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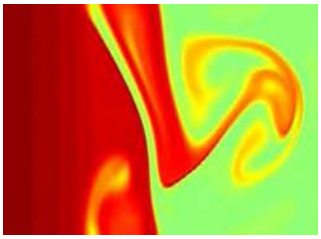
With increasing energy demands and a limited supply of fossil fuels, the need for efficient, clean, and sustainable energy sources grows ever more pressing. Nuclear fusion – the process from which stars like the Sun derive their energy – holds the potential to help address this challenge. To mimic this process on earth, experimental fusion devices seek to confine and heat gas to millions of degrees (creating a *fusion plasma*). Learning how such plasmas behave is a crucial step towards realizing fusion as a sustainable energy source. At the Plasma Physics and Fusion Energy (PPFE) section at DTU Physics, we are exploring this issue, focusing on three areas of high priority on the way towards a working fusion power plant:

1: We operate equipment to **measure key properties of fusion plasmas** in experimental devices such as *ASDEX Upgrade* in Germany. Using a technique called collective Thomson scattering (CTS), we can infer the density and dynamics of ions in the plasma. Monitoring of this is vital for achieving a high fusion output in future power plants.

The ASDEX Upgrade fusion device, with hot plasma glowing in pink

2: We are developing **simulations of plasma turbulence and particle transport** in fusion plasmas. These issues play a key role in determining overall plasma behavior and how well the plasma remains confined in the fusion device. Understanding this is important for optimizing plasma performance and for controlling its heat exhaust.



Simulated turbulent plasma structures in ASDEX Upgrade

3: We are also **designing CTS equipment for the next-step fusion device *ITER***, in which plasma temperatures will exceed 200 million C. This machine is currently being built in France in a large international effort to experimentally demonstrate fusion as a viable energy source and pave the way for the first fusion power plant.

Sketch of ITER (currently being built). Note person circled in red at bottom left

H_2CAP - Hydrogen assisted catalytic biomass pyrolysis for green fuels

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Fast pyrolysis of biomass produces a high yield of bio-oil through well-established technologies [1]. To utilize this oil as liquid fuel the oxygen content must be reduced from 35-50 wt.% down to <1 wt.%, which increases heating value and stability and decreases acidity [1]. Upgrading bio-oil by catalytic hydrodeoxygenation (HDO) is challenged by severe polymerization and coking upon heating the oil. Alternatively, performing fast pyrolysis in high-pressure hydrogen atmosphere in a fluid bed reactor with a HDO catalyst as bed medium, could immediately stabilize reactive pyrolysis vapors [2]. An additional vapor phase HDO reactor could ensure removal of oxygen down to <1 wt%, resulting in separate hydrocarbon oil and water phases being recovered. A simplified bench scale setup of this process has been constructed at DTU Chemical Engineering. With a capacity of 100 to 300 g/h solid biomass, the aim is to provide a proof-of-concept for the continuous conversion of solid biomass to low oxygen, fuel-grade bio-oil.
Experiments were performed with 50 g of $CoMo/MgAl_2O_4$ catalyst in the fluid bed reactor and 173 g of $NiMo/Al_2O_3$ catalyst in the HDO reactor. The catalysts were sulfided before experiments. Hydropyrolysis of beech wood was performed at 25 bar with gas composition 470 ppm H_2S, 6 % N_2 balance H_2. A photograph of the condensed liquids from Exp. #4 and the yields obtained from Exp. #1 to #4 are shown in Figure 1.

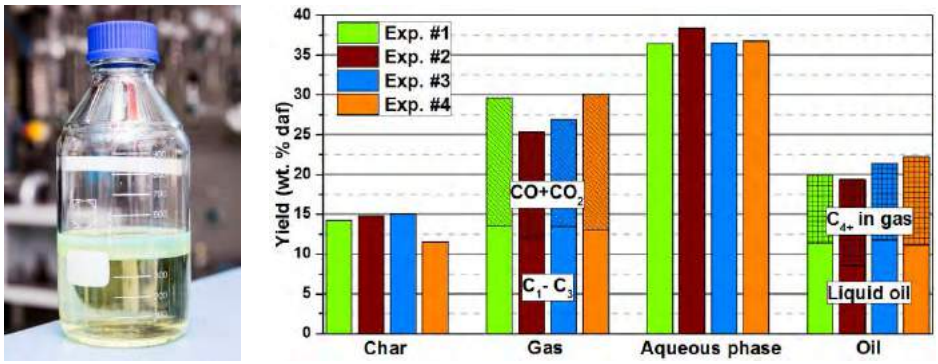

Figure 1: Photograph of the recovered liquids from Exp. #4, oil is top phase. Yields of char, C_1-C_3 hydrocarbons, CO + CO_2, condensed aqueous phase and condensed oil with potentially condensed oil (C_{4+}) in gas phase on dry, ash free basis for Exp. #1 to #4. The mass balance sum to 100, 98, 100 and 101 % respectively.

These very first results show that the process performs excellently as intended. The products are phase separated aqueous and hydrocarbon fractions. The low viscosity, free-flowing oil with <1 wt.% oxygen is very different from conventional wood pyrolysis oil. The best oil yield obtained is 22.2 wt.% of the wood, corresponding to approximately 39 % carbon atom yield and an energy yield of approximately 53 %. The liquid yield may be further improved by choice of catalysts and reaction conditions, which is the focus of ongoing work.
This study confirms that catalytic hydropyrolysis with hydrodeoxygenation is an attractive route for biomass to liquid fuels. The reaction conditions employed are significantly milder than gasification, potentially resulting in lower capital and operating costs, and the energy yield is significantly better than 2nd generation bio-ethanol.

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Developing diagnostic systems for ITER – the next step fusion energy experiment

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Fusion energy research is moving to the next stage with the well progressed construction of one of the largest research infrastructures ever – ITER. The goal of ITER is to produce 500 MW of fusion power while heating the fuel – deuterium/tritium plasma – by 50 MW. This will confirm fusion energy to be a viable energy source. Fusion energy power plants will be safe and can be operated to supply the baseload of an energy system. The fuel resources are inexhaustible, and can be derived from sea water. Fusion energy is based on the nuclear reaction fusing hydrogen isotopes into helium – like in the Sun – and thus no CO_2 is released in the energy production. The waste of the energy production is the irradiated steel of the core of the reactor, but this radioactivity will only last for about 100 years and no long-term radioactive waste storage is needed.

While the promise of safe, clean and abundant energy is the ultimate goal of fusion energy, the path towards this is challenging. A fusion plasma has a temperature of 200 mio. degrees (15 times that of the core of the Sun), and this is confined by a magnetic field generated by powerful superconducting magnets in a vacuum chamber of 1000 m^3. Operating diagnostic systems in the environment of ITER is a challenge for many technologies, but due to robustness, microwave diagnostics will play an increasingly important role in burning plasma fusion energy experiments like ITER and beyond. The Collective Thomson Scattering (CTS) diagnostic to be installed at ITER is an example of such a diagnostic with great potential in present and future experiments. The ITER CTS diagnostic will inject a 1 MW 60 GHz beam of electromagnetic radiation from a gyrotron into the ITER plasma and observe the scattering off fluctuations in the plasma – to monitor the dynamics of the fast ions generated in the fusion reactions. This will provide important physics understanding of the behavior of the fusion plasma that can be used for optimizing future fusion power plants.

A research team at DTU (DTU Physics and DTU Nutech) has been tasked by Fusion for Energy (the European coordinator for supplies to ITER) to develop the ITER CTS diagnostic in collaboration with Instituto Superior Técnico in Portugal. It is a 5 year effort of more than 50 man year total effort. This presentation will outline the prospects and the status of the development of fusion energy research and the CTS diagnostic system for ITER.

How should we fuel future fusion power plants?

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Future fusion power plants offer a cleaner, safe and sustainable source of electric energy. This can be obtained by fusing light nuclei in a reactor by processes similar to those in the Sun. The most promising design for such device is a *tokamak*, in which a plasma of hot hydrogen isotopes is confined by a toroidal magnetic field.

During operation the plasma requires refueling due to depletion of the original fuel by the fusion processes, and loss of heat and particles caused by outwards transport across the plasma edge. The transport from the edge region is strongly intermittent, and dominated by field-aligned filaments (blobs) [1]. A snapshot from a computer simulation of a blob event is shown in Figure 1.

Present and future tokamaks, such as ITER [2], are mainly fueled by the so called *gas puffing* technique, where neutral gas at room temperature is injected into the bulk plasma where it is ionized and thus confined. However, to reach the confined region the neutral particles must cross the region of open magnetic field lines outside the edge. If a neutral particle is ionized, for example by a blob, in this region, it will not contribute to the fueling.

It is investigated numerically how the plasma source profile from ionization of gas puffed neutrals is affected by the presence of blobs. This allows for estimating realistic ionization source profiles, and thus asses viable fuelling techniques for future fusion devices such as ITER.

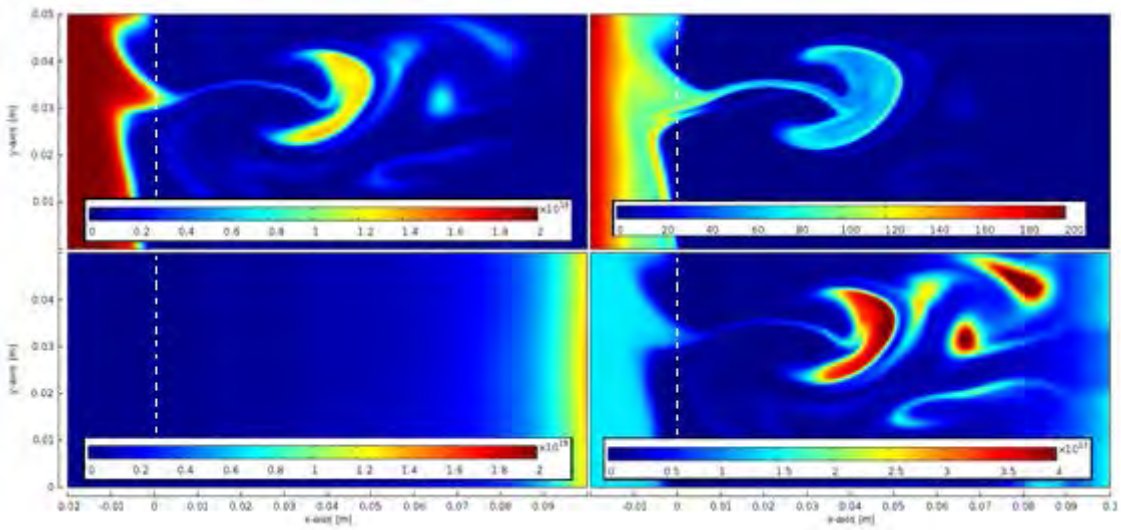

Figure 1: Simulation of the **(a)** electron density $[\mathbf{m^{-3}}]$, **(b)** electron temperature $[\mathbf{eV}]$, **(c)** neutral density $[\mathbf{m^{-3}}]$, and **(d)** ionization rate $[\mathbf{s^{-1}m^{-3}}]$ during a blob event. The simulated domain is a 2D slab perpendicular to the magnetic field lines, near the edge region of a tokamak fusion reactor. To the left of the dashed line is the region of confined plasma.

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Flavins mediate extracellular electron transfer in Gram-positive *Bacillus megaterium* strain LLD-1

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Electrochemically active microorganisms are microbes which can transfer electrons from cell to extracellular electron acceptors such as minerals, contaminants, electrodes, etc., and these processes are defined as extracellular electron transfer. In this study, we isolated and identified a new electrochemically active strain of *Bacillus megatherium* strain LLD-1, and its extracellular electron transfer mechanism was demonstrated by cyclic voltammetry (CV), differential pulse voltammetry (DPV), HPLC, and chronoamperometric.

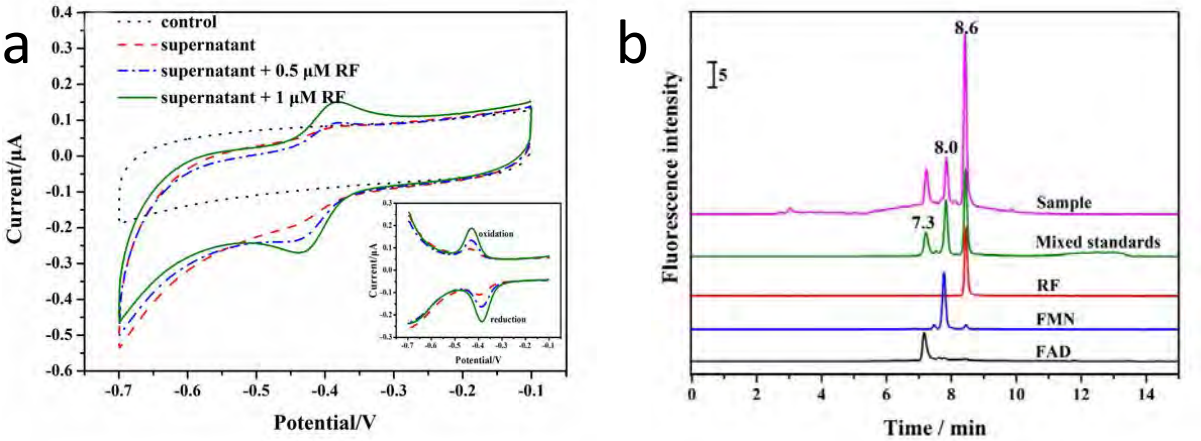

Figure 1 (a) CVs for the bare GC electrode in the 0.05 M PBS solution (control), in culture supernatant and in the presence of 0.5 and 1.0 μM RF; and the corresponding DPV assays was in the inlet. (b) The HPLC chromatograms for the single, mixed standard solution and sample (culture supernatant) collected at 36 h cell-culturing.

The CV and DPV showed that a redox peaks ascribing to membrane proteins was found in the strain LLD-1; another redox peaks observed in cell and supernatant were ascribed to flavins. 74% increment of voltage generation in LLD-1 inoculated microbial fuel cell (MFC) can be made by adding extra 0.1 μM flavins mixture solution.

Acknowledgments
This study was supported by grants from the National Natural Science Foundation of China (Grant No. 51208490; 51478451), the Knowledge Innovation Program of the Chinese Academy of Sciences (IUEQN201306) and Carlsberg Foundation (CF15-0164).

MEMS Inductor for Power Systems on Chip (PwrSoC)

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Power converters are the key driver in development of sustainable energy. They are the essential parts in most of electronic devices e.g. consumer electronics, LED lighting, and internet of things (IoTs). Lighting accounts 1/6 to 1/5 of global energy consumption [1] with around 10% loss in power supplies. Therefore, efficiency and size of power supplies plays an important role in reducing the amount of energy used. Smaller power supplies mean less raw materials used and more space for more functionality. Power systems on chip (PwrSoC) is the future envision of highly miniaturized SMPS where integrated magnetics is one key technology [2]. DTU Danchip and DTU Elektro and six industrial partners have been working on TinyPower project [3] focusing on PwrSoC technology for IoTs and LED drivers ($220V_{AC}$-$12V_{DC}$, 1A).

This work focuses on microelectromechanical systems (MEMS) air-core inductors for PwrSoC switching at very high frequency (30MHz – 300 MHz) range. A new architecture of 3D air-core toroidal inductor has been proposed (Fig. 1a) for low loss, reduced parasitic capacitance and minimal electromagnetic interference (EMI). We develop a CMOS-compatible, scalable and universal fabrication process based on cleanroom fabrication technologies. The process consists of three main stages [4] (Fig. 1a). They are (i) create through-silicon vias (TSV) by deep reactive ion etching (DRIE), (ii) electroplating of copper as conductive materials, (iii) remove the excess silicon core by DRIE to realize air-core inductors. Inductors were fabricated with scalable sizes (1mm^2 to 25 mm^2) and versatile geometries (Fig. 1b) e.g. toroid, transformer, solenoid, spiral, and advanced inductors that are impossible to make by wire-winding technology. As all process temperatures are kept below 200 ^{o}C, the inductors can be integrated into CMOS wafers by MEMS post processing. Toroid inductor (4 mm^2, 20 turns) showed peak Q-factor of 11.5 at 80 MHz with the inductance of 43 nH (Fig. 1c). This toroid is demonstrated in a 100 MHz resonant converter.

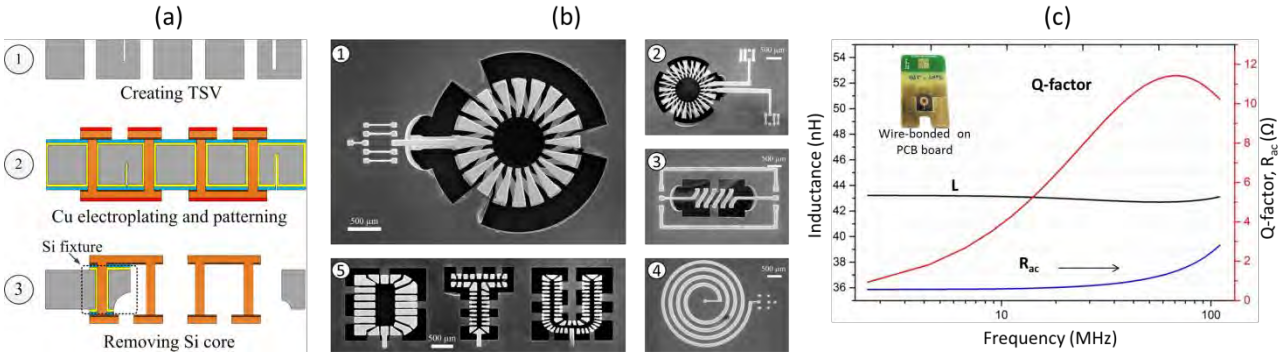

Figure 1. (a) Fabrication process, (b) fabricated inductors and (c) measurement results of a toroid inductor.

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The nexus between energy, climate change and sustainable development: Interlinkages between the Mexican NAMA for sugar mills and the SDGs

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The first half of 2016 was the planet's warmest half-year on record and without additional mitigation efforts, the global mean surface temperature may increase between 3.7°C and 4.8°C by 2100 [1] [2]. Some experts agree that any level above 2°C would mean impacts incompatible with sustainable development and will make it harder to achieve objectives such as food and livelihood security, poverty reduction, health or access to clean water [3]. In order to significantly reduce these impacts, it is urgent to accelerate the implementation of mitigation actions, which in many cases are nested in decision processes outside a distinct climate policy sphere. Particularly the energy sector holds a large mitigation potential; the decarbonization of electricity generation has been identified as a key component of cost-effective mitigation [4]. Bioenergy is an option that can contribute to shift society's dependence away from fossil fuels in the short and medium terms; however, there is still limited scientific basis regarding its interactions with sustainable development [5] [6] [7]. Depending on factors such as the technology used; the location, scales and pace of implementation; the land category used; the governance systems and the business models adopted, bioenergy implementation, can either generate co-benefits or adverse side-effects impacting sustainable development [8] .

The recognition of the interrelation and interdependence links between climate change, sustainable development and energy, calls for the creation of integrated strategies with a view of long-term effectiveness [9]. In this work, I am looking at the specific case of the National Appropriate Mitigation Action (NAMA) for sugar mills in Mexico, a climate policy instrument aiming to speed up investments in energy efficiency and co-generation infrastructure in sugar mills to maximize efficient clean electricity generation from sugar cane bagasse. Potentially this instrument will additionally enable the use of other agricultural residues that are currently being burned in open fields after harvest [10]. Besides, contributing to climate change mitigation through the displacement of carbon intensive electricity generation, other expected future sustainable development impacts have been identified through the application of an ex-ante qualitative assessment following the framework for measuring sustainable development in NAMAs suggested by Holm, et.al. [11], which consider environmental, social, economic and institutional aspects. Expected future impacts of the NAMA for sugar mills in Mexico include improvement in air quality arising from the reduction of black carbon and other air pollutant emissions, increase share of renewable energy in the energy mix, promote the investment in energy infrastructure and clean energy technologies, contribute to achieve higher levels of economic productivity through diversification, technological upgrading and innovation, improve energy efficiency rates, and support job creation. Additionally, if it enables the use other agricultural residues, it can provide an additional source of income for smallholder farmers and encourage the creation of micro-, small- and medium-sized enterprises in rural areas. Further research is needed to quantify these expected benefits and to develop a measuring, reporting and verification system to assess the efficiency of the policy instrument in achieving the expected goals.

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Selective H_2S removal from bio-methane gas by ionic liquid technology

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Biogas production in Europe has increased exponentially over the last decades, see figure 1. Raw biogas consist of roughly 60 % methane, 29 % CO_2 and 1 % trace gases of which hydrogen sulfide (H_2S) is the most problematic because of its toxicity and corrosive nature [2]. Upgrading of biogas by removing acidic components (CO_2, H_2S) by amine scrubbing processes is possible but expensive. Therefore, the prevalent usage of biogas is direct (on-site) combustion to generate electricity and heat. In order to avoid SO_2 emissions in direct combustion, H_2S needs to be selectively separated from the raw biogas.

Recently, dual lewis base (DLB) ionic-liquids (ILs) have been reported to capture H_2S very efficiently, selectively and reversibly [3]. The high efficiency and selectivity is ascribed to the nitrogen atom of the anions. However, the reported ILs suffer from high viscosity and probably low stability of the ammonium based cations.

Our current research project aims at alleviating these two problems by preparing nicotinate (NIA) based ILs with other cations such as phosphonium and imidazolium based ones. Furthermore, we will try to prepare monolithic samples containing the best ILs in order to be able to test them under real conditions.

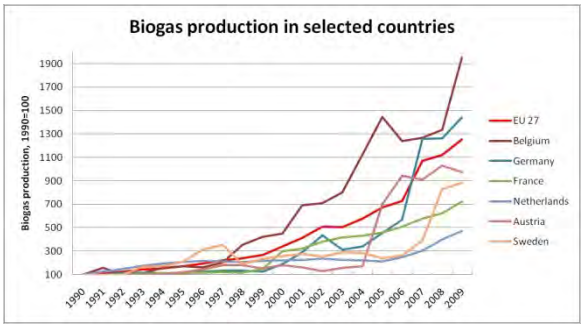

Figure 1: Biogas production from 1990 to 2009 in selected countries [1].

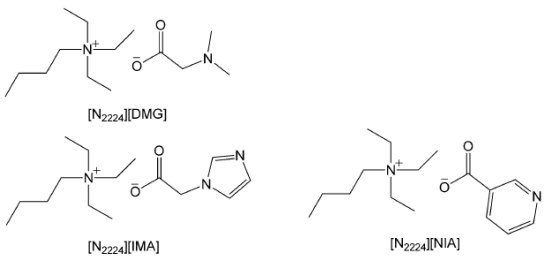

Figure 2: Structures of promising ILs [3]

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Title:

Dynamic reaction phenomena during electrochemical reduction of CO on size selected copper nanoparticles

Abstract:

Reduction of CO2 to higher hydrocarbons is important for closing the carbon cycle and providing a sustainable production of industrial chemicals and fuels for the future. Furthermore, being able to do this electrochemically decreases both capital investment and opens the possibility for decentralization, redundant facilities and on-demand production. To date, the best candidate for electrochemical reduction of CO2 to hydrocarbons is copper, which has been studied in detail since 1985[1], but despite several decades of research in this field, the catalytic pathways for this reaction are not yet well understood.

Using a highly sensitive instrument for real-time electrochemical mass spectrometry (EC-MS) [2], we have investigated CO electroreduction on size-selected copper nanoparticles, focusing on the dynamic behavior of hydrocarbon formation at the onset of CO electroreduction as a means to gain insight into reaction mechanisms. For the first time, we observe a high rate of methane production at the onset of constant-potential CO reduction which is decoupled from the production rates of hydrogen and ethylene. The methane production comprises of two separate parts: a dynamic contribution at the onset of the experiment roughly corresponding to the desorption of a single monolayer, and a subsequent steady-state production. Quantifying these two parts independently, it is clear from the potential dependence, i.e. Tafel slopes, that dynamic CH4, steady CH4, steady C2H4 and steady H2 all follow different catalytic pathways. Furthermore, we show that the dynamic methane depends on exposing the electrode surface to air-saturated electrolyte prior to electrolysis while the electrode is held at a potential anodic of RHE, indicating that surface oxygen activates a catalytic pathway to methane. In addition to providing mechanistic insight, this result suggests a new strategy for increasing Faradaic efficiency of CO reduction to hydrocarbons, by stabilizing or regenerating metastable pathways.

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Authors:

Søren B. Scott, Daniel B. Trimarco, Anders Bodin, Nicola Mazzanti and Ib Chorkendorff

Open Data and Open Source as a precondition to meet challenges in modelling sustainable energy systems

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The transformation to sustainable energy systems is necessary to meet climate change ambitions and Sustainable Development Goals. Due to the complexity of interlinked energy systems, computer models are required for assessing optimized system configurations from a social economic point of view while meeting the precondition of emission reduction goals. Although results of these calculations are highly dependent on input data, code and scenario assumptions, it has been common praxis to publish only results (Cao et al 2016).

With the objective to meet the scientific principle of reproducibility, the whole process of choosing original input data, making assumptions, processing data, writing code and post-processing of result data has to be made openly available. This enhances on the one hand quality, scientific soundness and transparency (Wiese 2014) and on the other hand increases efficiency and faster progress regarding questions on how to design sustainable energy systems as double work can be avoided and model parts can build upon each other. Furthermore, well established open licenses on data and code can create legal certainty as the common praxis of openly available data utilized in energy system models is in many cases not defined clearly (OPSD 2016).

Research on current challenges of modelling sustainable energy systems revealed that Open Data and Open Source is a precondition but no warranty for reproducibility, efficiency and scientific soundness (Wiese 2016). Development on open standards, data management, documentation of large data sets, modular structure, collaborative code development and well-defined interfaces are required.

The presentation will give an overview on current developments of Open Source and Open Data in energy system research and discuss its contributions to the challenges of energy system modeling as well as remaining challenges.

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Micro-CT in-situ experiments to investigate the development of high-porosity channels in chalk sample for CO2 storage

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Carbon capture and storage is critical to the remediation of global climate change induced by the development of fossil fuel industry. One of the key methods for carbon storage is to inject CO_2 into geologic settings such as chalk reservoirs in the North Sea. During the injection process, chalk dissolution has two major impacts. In one hand, chalk dissolution creates more pore space for CO_2 trapping. However, it also deteriorates the rock strength and could potentially cause collapse. Finding an effective way to create more pathways for CO_2 dissipation while maintaining the stability of the rock layer is crucial for the implement of CO_2 injection. X-ray imaging is an effective non-destructive tool for material study. This study applies micro-CT in-situ experiments to observe the effects of flow rate on chalk dissolution and porosity development. Deionized water was used to minimise the size of developing pores. In another experiment which CO_2-enriched water was injected under various conditions of pressure and temperature, parameters such as the pressure drops across the samples are measured. From these parameters, we can evaluate the changes in porosity and permeability due to the dissolution of calcite.

Socio-Economic costs of cooking fuel in Refugee Camps in Tanzania

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In Northwest Tanzania, 180,000 new refugees have arrived since 2015, total refugee population in camps reaching 240,000 in October this year (UNHCR, 2016). The majority of households in the Tanzanian refugee camps use firewood or other traditional biomass for cooking. Firewood does not carry any direct financial cost as it is collected in the nearby areas. However, the use of firewood for cooking has a negative impact on the local environment, human health, and has substantial economic cost (due to loss of productive time), especially affecting women and girls (Lambe et al., 2015). In a refugee setting, collecting firewood can contribute to conflicts with local populations due to resource scarcity.

This study aims to demonstrate the complete costs, including social and environmental externalities, of current technologies and fuels used in refugee camps in Northwest Tanzania and compare these with the alternatives. The analytical basis provided by this study can be used to facilitate investment to help diffuse more sustainable energy technologies for cooking in refugee camps.

Present energy consumption patterns and technologies will be used to determine the level of demand in terms of resource and embedded energy. Indoor air pollution data will be used for assessing health impacts. To determine the extent of deforestation, aerial photographs/GIS data will be compared and analysed alongside known estimates of tree-cover loss based on firewood consumption in the area. Economic details, including population size, incomes, time used to obtain cooking fuel will be used to determine the potential loss of income-generating time and time spent in education. The current status will be compared with possible technology and fuel alternatives.

Figure 1: Cooking technology alternatives in rural setting: a biogas stove & an improved woodstove.

Early results from the UNHCR background study indicate that Liquid Petroleum Gas (LPG) may be a viable alternative, which would save more than 160,000 tonnes of firewood across the camps in Northwest Tanzania.

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Multi-purpose In Situ TEM holder for Characterization of processes for Energy Storage.

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1: DTU CEN; 2: DTU Nanotech; 3: DTU Physics

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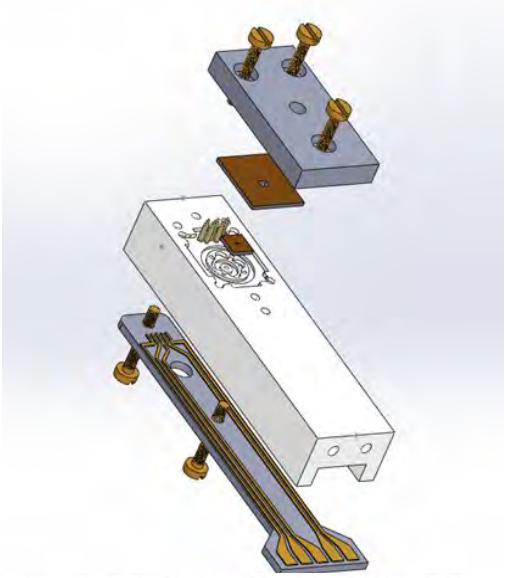
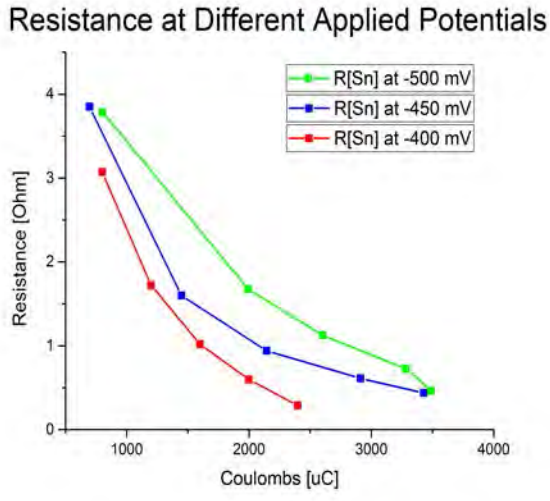
The rapidly growing energy demand around the world is driving the development of sustainable alternative energy sources. This in turn drives the need for energy storage where batteries have the possibility to solve this problem, when better understanding of the fundamental obstacle for improvements have been reached. In Situ liquid cells for electron microscopy and x-ray tomography of a processes in liquids one very promising and emerging technology for fundamental research of battery materials and processes. Our team have produced a multitude of holder system for analysis with TEM, SEM and CT instruments. This systems are all based on the same chip design, that forms the transparent closed cavity for the in situ experiments. This makes it possible to run the many different analysis in the same reference system.
We demonstrate the following concepts:

- Low cost multipurpose, holder for SEM and x-ray CT
- Using tin as an example material that can be lithiated, we show In situ electroplating of smooth tin layer on micro electrode
- In situ 4-point condoctivity measurements of deposited tin layer
- In situ STEM in SEM
- Holder compatibility with LiPF6



On of the major goals was to develop the 4-point measurement of an electroplated tin layer. These measurements have been show at different depositing potentials with subsequencet stripping on the same electrodes, see graph.



The flow capabilities of the systems allowed for the us of LiPF6 DMC/EC as and electrolyte for creating a near comocial system in our holders.

This project can thus i large contribute to ther future understanding of fundamental for battery technologies.

Structure – Activity – Stability Relationship of Nanostructured Model Electrodes

Albert K. Engstfeld[1]*, Thomas Maagaard[1], Sebastian Horch[1], Sylvain Brimaud[2], R. Jürgen Behm[2], Ifan E.L. Stephens[1] and Ib Chorkedorff[1]

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Catalysts are of huge interest for economic and environmental applications. They are in almost every industrial process involving chemical production. They play an important role in the field of energy conversion and storage, such as fuel cells or electrolyzers. In order to improve catalyst performance, atomic scale knowledge of the catalyst structure and the interplay between the reactants, reaction intermediates and products is mandatory. Industrial catalysts consist of single metal or alloy nanoparticles supported on a complex three dimensional high surface area carbon or oxide support. In this case the reactivity strongly depends on the structural properties of the supported particles, which change with the size, morphology and the composition of the particles (in the surface and in the bulk). They can furthermore be influenced by the interaction with the support.

One approach to disentangle all these effects involves investigations on well-defined planar model systems. Experimentation on such structures became available with the introduction of ultra high vacuum (UHV) surface sensitive techniques; they allows for the elucidation of the structural, electronic, and chemical properties of the prepared surface structures.[1] Over the last decades a vast number of efforts have been made to prepare and characterize a huge number of nanostructures, primarily based on scanning tunneling microscopy studies, which allow for atomic scale characterization of structural elements of metal electrodes.[2] If we think about a conceptual design to prepare model catalysts, where the experimentalist becomes a designer rather than an observer, we can make use of these existing tools to prepare very specific bimetallic nanostructured electrodes on an atomic scale level. Combining UHV techniques with an electrochemical cell, where controlled contamination free transfer conditions between both techniques is ensured,[3] allows for a direct correlation between structural and catalytic properties. It sheds light on restructuring processes occurring on the surface during the electrochemical reaction.[4] On the basis of this insight we can develop new strategies for improving catalyst performance.

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THERMCYC – Advanced Thermodynamic Cycles Utilizing Low Temperature Heat Sources

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The current paradigm of a sustainable society requires not only a shift to renewable energy supply, but also an efficient use of energy. In this context, the THERMCYC project aims at utilizing low temperature heat sources potentially available in Denmark, such as waste heat from the industry and transport sector. These sectors account for 64 % of an estimated 212 PJ of low temperature waste heat in Denmark [1], representing a large resource, which can significantly contribute to the reduction of the primary energy demand. State-of-the art technologies for waste heat recovery (WHR) can be improved by advanced cycle and components design, and the use of multi-component working fluids. The project focuses on devising heat pump solutions for high temperature heat production and organic Rankine cycle (ORC) systems for electricity generation.

A first case study [2] investigated the integration of a heat pump in a spray drying facility utilizing zeotropic mixtures as working fluids. The unit was designed to recover waste heat at 68 °C for air pre-heating at 120 °C. Figure 1 shows the heat pump cycle using a mixed refrigerant and accordingly improving the match of the temperature profiles in the heat exchangers. The selection of a suitable working fluid enhances the thermodynamic and economic potential and represents a feasible solution, leading to a 36 % reduction of the natural gas consumption.

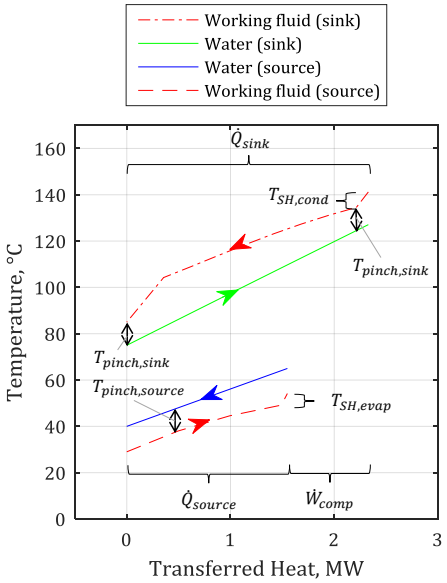

Figure 1: T-$\dot{Q}$-Diagram of a heat pump for WHR of a spray drying facility

A second case study [3] investigated the waste heat recovery from the jacket cooling system of a diesel engine aboard a large marine vessel. The fuel consumption of the ship was reduced by using an ORC unit. The system design was optimized for a number of multi-component working fluids, in combination with the design of the turboexpander. The results indicate that the unit can provide 200 kW of additional power with the pure fluid R245fa and constrained engine operation, whilst the mixture R245fa/n-pentane provided around 444 kW when the water temperature was not constrained.

The presented cases document the significant potential of waste heat utilization by minimizing entropy generation due to various irreversibilities related to component design and working fluid properties.

[1] Bühler F., Holm F. M., Huang B., Andreasen JG. and Elmegaard, B. (2015), Mapping of low temperature heat sources in Denmark Proceedings of *ECOS 2015: Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems*

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Session

F

Oral Presentations

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UniProtein®, a novel protein product

Eleni Ntokou[*1]

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Imagine a future where the world's protein supply is partly covered by a fermentation technology that decouples protein production from farming and fishing by enabling methane to be turned into protein. Unibio owns the rights to a disruptive bioindustrial and highly scalable protein production technology, the U-Loop® technology, that converts carbon from methane into a high-value bacterial protein product, UniProtein®.

Unibio's proprietary U-Loop® fermentation technology is based upon a process occurring in nature and allows the production of safe, stable and affordable high-quality feed protein without any of the environmental issues of overfishing, deforestation, pollution of water and use of pesticides and fertilizers. Basically, agricultural land and fisheries can thus, to a much larger extent, be reserved to produce human foods instead of being utilized to produce protein to husbandry and meat product production. This would also in turn put less stress on e.g. rain forests as the need to clear forests to produce soy could be reduced.

The methanotrophic bacterium *Methylococcus capsulatus,* that Unibio uses to produce UniProtein®, requires a system capable of handling a large volumetric gas fraction while providing a high gas-to-liquid mass transfer. The U-Loop® fermentor is different from existing forced-flow recirculation loop systems. In the U-Loop® fermentor gas and liquid are mixed by pumping gas and liquid through a vertical U-shaped pipe fitted with static mixers. Mixing time decreases and mass transfer increases with an increasing volumetric liquid flow rate and specific power input. Very large mass transfer coefficients, considerably higher than those obtainable in a stirred tank reactor and previous tubular loop reactors, can be achieved in the U-Loop® fermentor equipped with static mixers at modest volumetric liquid and gas flow rates[1]. The technology has been developed in close collaboration between Unibio and the Technical University of Denmark (DTU), and the testing and development of the protein product are being performed in close collaboration with the animal science department of Aarhus University (AU).

Unibio's technology is currently being used to produce UniProtein® in Denmark, an EU approved bacterial protein meal for animal nutrition. UniProtein® addresses the world's growing need for animal protein, a need that will continue to grow in line with population growth and the emergence of a large middle class with strong purchasing power, which has increased the demand for meat products. UniProtein® is a protein-rich biomass (72.9% protein) and can be used as a direct supplement in animal feed compounds. It has a long shelf life, and the production process always results in a uniform product. UniProtein® is a non-polluting product, as it is produced by a microbial culture with natural gas as the sole carbon and energy source. The only waste product from this production is clean water. The product is free from toxins, dioxin and heavy metals due to the controlled production process and the fact that all minerals used are food grade.

In the long term, Unibio intends to improve the end-product of its U-Loop® technology regarding the following aspects: increased protein content, nucleic acids, use of the product as an intermediate.

Session

F

Laptop Presentations

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Development of smart molecularly imprinted polymers for use in sustainable food nanosensors

Dr. Jon Ashley[1], Associate Professor Yi Sun*[1]

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In this project we aim to develop core shell imprinted polymers for use in microfluidic based biosensors. By combining the magnetic properties of iron oxide for facile sample preparation, the fluorescent properties of quantum dots as the optical transducer, as well as molecularly imprinted polymers as the receptor, an optical based biosensor will be developed, capable of detecting antibiotic residues in pork products. Iron nanoparticles and CdTe quantum dots were synthesized using standard synthesis protocols. The resultant Fe_3O_4 nanoparticles were treated with tetraethyl orthosilicate (TEOS), and the CdTe quantum dots were then encapsulated. Finally a thin MIP layer was polymerized round the nanoparticles using azobisisobutyronitrile (AIBN) as the initiator, ethylene dimethacrylate (EDMA) as the crosslinker, acrylamide (AAm) and methacrylic acid (MAA) as the monomers and the antibiotic as the template. By incorporating a microfluidic based platform with the developed smart nanomaterials, a handheld sensor capable of multiplex detection will be developed. It can be used within a food manufacturing environment for the routine screening of pork products and provide a more sustainable replacement for animal derived antibodies.

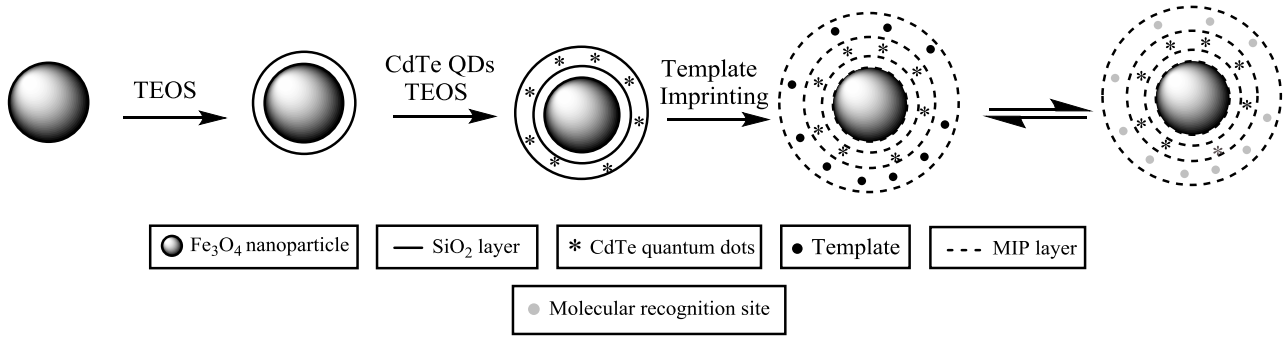

Figure 1. Overview of the synthesis strategy for the development of the multifunctional nanoparticle sensor.

The effect of added enzymes on process potentials derived from different qualities of barley: a model study using simulated mashing conditions by rapid visco analyser

Radhakrishna Shetty, Shiwen Zhuang, Rasmus Lyngsø Olsen, Preben Bøje Hansen and Timothy John Hobley*

Barley sorting is an important step for picking up grain of desired quality. Whilst brewing with 100 % sorted barley (picked high quality) has become realistic with the addition of exogenous enzymes, the effect of added enzymes on process potentials derived from un-sorted barley (mixed) and sorted-out barley (low quality) were almost not investigated. The aims of this study were to examine the rheological behaviours of sorted out barleys affected by addition of enzymes in comparison with sorted barley, and to evaluate the quality attributes derived from respective barleys focusing on wort fermentabilty and filterability parameters. To achieve this, rapid visco analyser was used to simulate brewery mashing process by applying two commercial enzymes (Ondea® Pro and Cellic® CTec2) at lab scale. During the simulated process, the rheological profile of low quality barley was markedly different from others, irrespective of enzyme type, whereas small difference was observed between the sorted and un-sorted barley. With respect to the major wort nutrients for fermentation, the sorted-out barley generated the lowest sugar yield, regardless of the enzyme used; however, the use of Cellic® CTec2 resulted in significantly higher sugar content compared to Ondea® Pro, irrespective of the quality types of barley. Interestingly, considerably higher levels of free amino nitrogen were observed resulting from the sorted-out barley, likely due to the smaller size/weight of the barley compared to others. For wort filterability, the Ondea® Pro treatment resulted in significantly lower turbidity and smaller particle size compared to Cellic® CTec2; however, this effect was observed in sorted and un-sorted barley but not in sorted-out barley. Consequently the un-sorted barley demonstrated great potential in brewing process with added enzymes, whereas the sorted-out barley is not comparable to sorted barley in terms of rheological behaviors of mashes, as well as nutrient and filtration parameters studied, showing potential as biofuel feedstock that can be degraded to fermentable sugars by enzymes such as Cellic® CTec2.

Session

F

Poster Presentations

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Food production viewed through the lenses of industry 4.0

Zaza Nadja Lee Hansen*[1], Peter Jacobsen[1]

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Industry 4.0 promises big changes for businesses in all sectors and of all sizes. In the coming years we will see an increasingly digital supply chain, smart production (e.g. increasing automatization and interconnectivity) and more digital and connected products and devices (see figure 1)

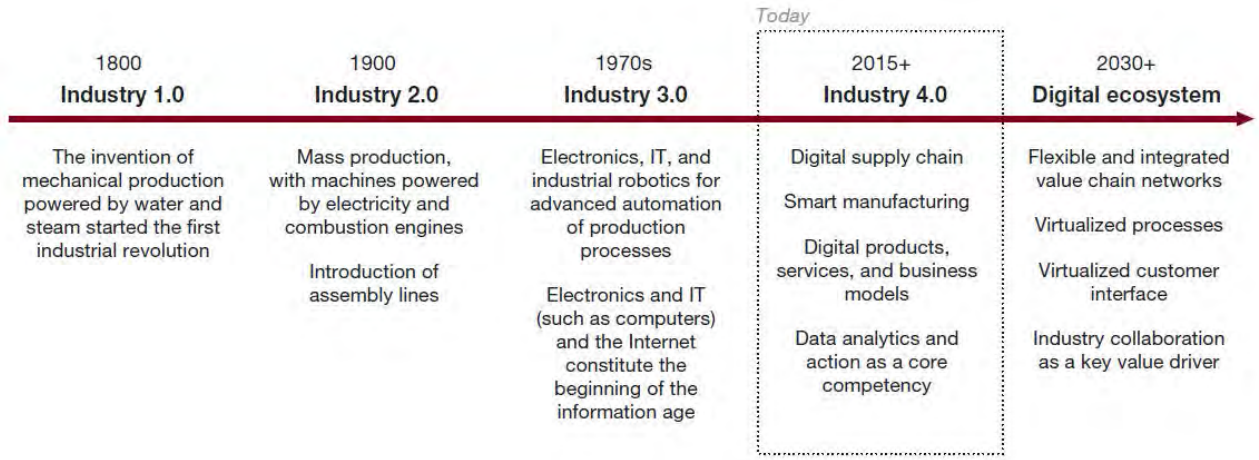

Figure: 1: Industry 4.0 (Source: PriceWaterhouseCooper)

These changes will give the food industry a new production paradigm; a new way of viewing itself in the larger supply chain and a new way to produce. However, new risks and challenges also needs to be considered. Some of the ideas we will present include:

1. What are the key benefits the food industry can gain from industry 4.0?
2. What are the main challenges for this industry with industry 4.0?
3. How can the industry address the challenges?
4. How can the industry best exploit the key benefits of this new industrial paradigm while keeping sustainability as a key goal?

The goal is to develop a framework food producers can use when they are faced with decisions regarding industry 4.0, so that they gain the most competitive advantage from these changes while making their productions more sustainable. We wish to test this framework in Danish food companies in order to ensure the framework can be used as a key strategic decision tool.

Value utilization of discarded fish livers for production of omega-3 rich oil

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The intake of long chain (LC) omega-3 polyunsaturated fatty acids (PUFAs), especially eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA), has been associated with several health beneficial effects. Thus, there is a demand for new methods to obtain high quality omega-3 rich oils and applications with omega-3 to increase the population's intake of the healthy omega-3 LC PUFAs.

Most of the fish caught in Denmark are slaughtered and rinsed immediately after catch, when the fishing vessel is still at the sea. When the fish is rinsed, the liver is discarded in to the sea. However, this practice has now been prohibited in the new EU legislation. Liver from fish has a high content of omega-3 LC PUFAs, i.e. EPA and DHA. This liver could be stored and used for production of oil rich in omega-3 and thus, create value from waste material.

The quality of the livers will affect the quality of the oil produced. Thus, a good quality of the waste material has to be preserved from catch to oil production. Parameters that can affect the quality of the liver from catch to oil production are storage condition and initial oxidation stage. The aim of this study was to evaluate the effect of storage conditions (iced and -18 ^{o}C) on board the fishing vessel on the oxidative quality of different cod species. Additionally, a systematic evaluation of seasonal variation in oil content, oxidation status and fatty acid composition was performed on different cod species.

Antioxidant Activity of Protein Hydrolysates Obtained from Common Carp (*Cyprinus carpio*) Discarded Roe

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Lipid oxidation represents a severe challenge in food engineering because it deteriorates quality of foods, especially those containing high contents of polyunsaturated fatty acids (PUFAs). One way to overcome this barrier is application of synthetic antioxidants such as butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT), propyl gallate (PG), and tertiary butylhydroquinone (TBHQ) in PUFA-rich foods. However, recently there have been concerns over health-related risks posed by these synthetic agents. Therefore, obtaining safe antioxidants from natural sources, especially those which are discarded with no use, with potency to retard lipid oxidation has gained sizable attention.

Therefore, the present study aimed at obtaining "green" antioxidants from discarded common carp roe via the so-called hydrolysis process by using alcalase and determining their antioxidant activity both *in vitro* and in food model systems. Four common carp roe protein hydrolysates (CRPH) obtained at different reaction times (i.e. 30, 60, 90, and 120 min) were assayed. *In vitro* antioxidant activity of the hydrolysates was measured through three different assays (i.e. DPPH radical scavenging, metal ion chelating, and reducing power). Furthermore, the oxidative stability of 5% fish oil-in-water emulsions containing or not the hydrolysates was investigated by monitoring their content of hydroperoxides and volatiles markers. The hydrolysates exhibited high DPPH radical scavenging activity and reducing power when compared to positive controls, i.e. BHT and ascorbic acid, respectively. However, Fe^{2+} chelating capacity of the hydrolysates was relatively lower than that of Ethylenediaminetetraacetic acid (EDTA), applied as positive control. The antioxidant activity of hydrolysates changed with DH and increased in a dose-dependent manner. Unlike CRPH-fortified emulsions, the emulsions without CRPH exhibited significantly increased peroxide value (PV) during the storage period ($p<0.05$), reaching from 4.7±0.1 at day 0 to 79.2±11.3 at day 7. Moreover, all CRPH-containing emulsions showed negligible amounts of most secondary oxidation products (e.g. 1-penten-3-one and (*E,E*)-2,4-heptadienal) when compared to the emulsion control at day 7. These results indicate that common carp roe protein hydrolysates exert antioxidant activity both *in vitro* and in fish oil-in-water emulsions, and can thus be considered as alternative antioxidants to the synthetic ones.

Spatial differentiation in environmental impact assessment: how to properly estimate impacts from agricultural use of fertilizers

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The Product Environmental Footprint (PEF) is recommended [1] to quantify sustainable production and consumption. PEF is the potential environmental performance quantified over the product's life cycle stages from a supply chain perspective. PEF quantification can be achieved with the Life Cycle Assessment (LCA) framework – the tool to identify environmental hotspots and mitigation options across complex product value chains [2]. It is essential to be able to compare PEFs across alternative supply chains, production methods, and origin countries. Spatially differentiated indicators of the disturbance to Ecosystem Quality are required to address PEF at the various life cycle stages and emission/consumption locations. Such indicators typically model the environmental mechanism(s) components, i.e. fate, exposure, effect, damage, within the LCA framework [3].

This communication addresses a method developed to derive a spatially explicit marine eutrophication indicator [4] – one of the most important impact indicators for agriculture production. Just as fertilizing agricultural crops results in enhanced plant growth and production, the surplus of applied nutrients constitutes an environmental emission that disrupts the natural cycles in water bodies. Marine eutrophication reflects the ecosystem response to an excessive loading of nitrogen (N) to coastal waters [4]. Current available and recommended impact assessment methods for marine eutrophication lie short in the ability to provide the necessary spatially differentiated information. This fact is caused by insufficient pathway coverage, low environmental relevance, or incomplete geographic scope, thus rendering a limited applicability. The newly developed LCA characterization factors [4] are available for 5,772 river basins of the world. Methods were compared to show the value of spatial differentiation to the sustainability assessment of agriculture production.

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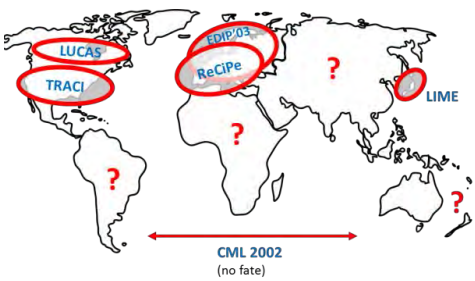

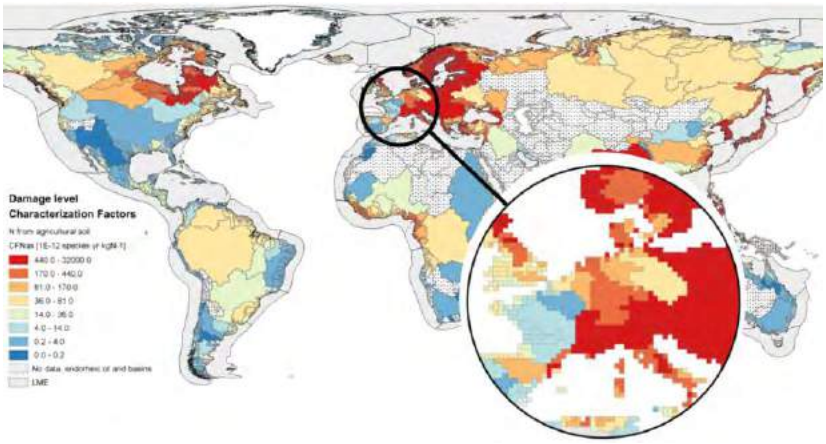

Session

G

Oral Presentations

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Session

G

Laptop Presentations

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Session

G

Poster Presentations

See session details and schedule on
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Session

H

Oral Presentations

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Whole genome sequencing for childhood cancer in Denmark

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Department of Bio and Health Informatics (DTU Bioinformatics)

The talk will describe our involvement in the Danish project STAGING, “Sequencing Three Actionable Genomes – Implications & National Guidelines”, an interdisciplinary, multi-tiered 3-year study of 600 consecutive childhood cancer patients and their families, with extensive genomic sequencing of host, tumour and gut microbiome’s genomes. In Europe, cancer accounts for approximately 25% of all deaths in children >1 year. Most cured patients are burdened by late effects, including risk of second cancer and debilitating toxicities. Recent advancements in genetic sequencing technology and reduction in costs have led to new strategies for identification of cancer predisposition and targeted treatment. STAGING is a nation-wide programme offering full, up-front genetic testing for childhood cancer patients and implements the findings into health care. Paediatric oncology provides a unique proof- of-principle framework for such a program, since it is one of the best organized medical specialties with nation-wide strategies for diagnostics, therapy, deep response phenotyping, and follow-up.

Curbing the development and spread of 'high risk' bacterial pathogens

Lars Jelsbak
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MDR (multi-drug Resistant) og XDR (Extensively drug resistant) Pseudomonas aeruginosa clone types spread at alarming rates in hospital environments, and there is a clear need to limit the development and spread of these 'high risk' bacterial pathogens. I will describe our recent efforts to use genomic information to determine the mechanism by which these clone types evolve and spread, and our work on the development a web-based tool that can make identification of high risk clones faster in the clinical microbiology hospital departments. The rationale behind the development of this tool is that faster diagnosis will help to improve containment of the pathogens.

Pyrolytic carbon electrode for dopamine detection from cells

Ada-Ioana Bunea*, Arto Heiskanen, Anders Kristensen, Stephan Sylvest Keller, Niels Bent Larsen and Jenny Emnéus

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Our group is working on the development of a carbon waveguide meant to be used as a new type of implant for patients with Parkinson's disease. The device would allow simultaneous monitoring of local dopamine concentration and controlled release of dopamine from cells upon light stimulation (Fig. 1).

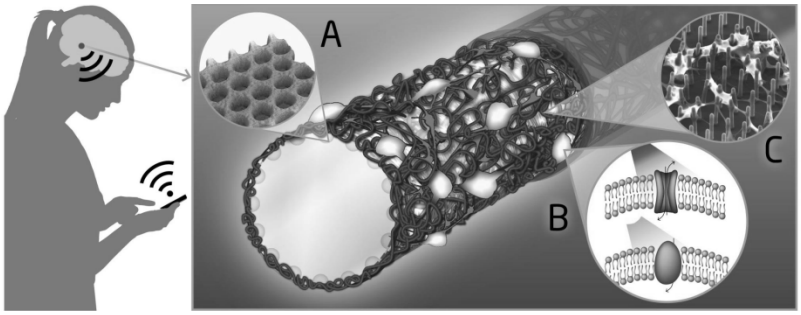

Fig. 1. Concept: Light travelling through the optical fibre is leaked to the surface (A) and stimulates the optogenetically modified cells growing on the carbon (B, C). The electrochemically active surface can be used for measuring dopamine exocytosis. The whole device could be implanted and controlled remotely.

We have previously shown that pyrolytic carbon surfaces enhance the differentiation of human neural stem cells into dopaminergic neurons [1]. Recently, we have been working on testing the electrochemical properties of pyrolytic carbon electrodes fabricated using polyimide as carbon precursor. The obtained electrodes show good reproducibility and electrochemical behaviour when tested with standard redox couples ($K_4[Fe(CN)_6]/K_3[Fe(CN)_6]$ and $[Ru(NH_3)_6]Cl_2/[Ru(NH_3)_6]Cl_3$) (Fig. 2A) and dopamine (Fig. 2B). For the detection of dopamine, the intensity of the oxidation peak shows a linear response to concentrations up to 200 µM, with a limit of detection below 5 µM (Fig. 2C). Thus, the electrodes could be used as cell culture substrates and to detect dopamine released from dopaminergic neurons grown on the surface.

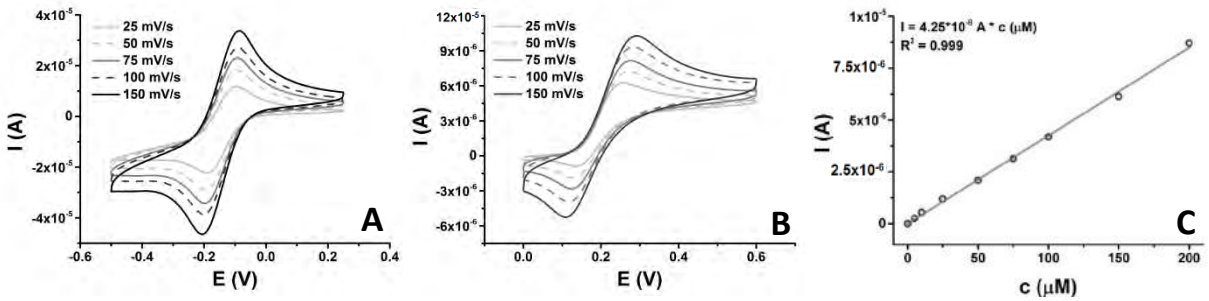

Fig. 2: Electrochemistry measurements: Cyclic voltammogramms at different scan rates obtained with 1 mM $Ru(NH_3)_6]Cl_2/[Ru(NH_3)_6]Cl_3$ (A) and 200 µM dopamine (B). Calibration curve for dopamine detection using the intensity of the oxidation peak from cyclic voltammetry (C).

References:

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* The device is currently being patented, application number EP16176841

Ranking factors involved in diabetes remission after bariatric surgery using machine-learning integrating clinical and genomic biomarkers

Helle Krogh Pedersen[1], Valborg Gudmundsdottir[1], Mette Krogh Pedersen[1,2], Caroline Brorsson[1], Søren Brunak[1,2] and Ramneek Gupta*[1]

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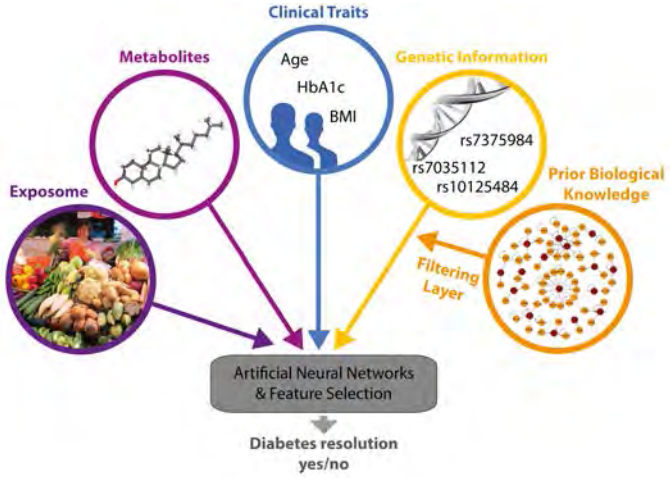
As weight-loss surgery is an effective treatment for the glycaemic control of type 2 diabetes in obese patients, yet not all patients benefit, it is valuable to find predictive factors for this diabetic remission. This will help elucidating possible mechanistic insights and form the basis for prioritising obese patients with dysregulated diabetes for surgery where diabetes remission is of interest. In this study, we combine both clinical and genomic factors using heuristic methods, informed by prior biological knowledge in order to rank factors that would have a role in predicting diabetes remission, and indeed in identifying patients who may have low likelihood in responding to bariatric surgery for improved glycaemic control. Genetic variants from the Illumina CardioMetaboChip were prioritised through single-association tests and then seeded a larger selection from protein–protein interaction networks. Artificial neural networks allowing nonlinear correlations were trained to discriminate patients with and without surgery-induced diabetes remission, and the importance of each clinical and genetic parameter was evaluated.

The approach highlighted insulin treatment, baseline HbA1c levels, use of insulin-sensitising agents and baseline serum insulin levels, as the most informative variables with a decent internal validation performance (74% accuracy, area under the curve (AUC) 0.81). Adding information for the eight top-ranked single nucleotide polymorphisms (SNPs) significantly boosted classification performance to 84% accuracy (AUC 0.92). The eight SNPs mapped to eight genes — *ABCA1*, *ARHGEF12*, *CTNNBL1*, *GLI3*, *PROK2*, *RYBP*, *SMUG1* and *STXBP5* — three of which are known to have a role in insulin secretion, insulin sensitivity or obesity, but have not been indicated for diabetes remission after bariatric surgery before.

In conclusion, we have proposed and applied a machine-learning based approach for ranking clinical and genomic features allowing non-linear combinations, in order to uncover factors at play in diabetes remission triggered by bariatric surgery. The general framework holds the potential to integrate additional data types, such as environmental factors or metabolite concentrations on an equal basis.



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Session

H

Laptop Presentations

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Session

H

Poster Presentations

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Electrospinning of Chitosan-Xanthan Nanofibers

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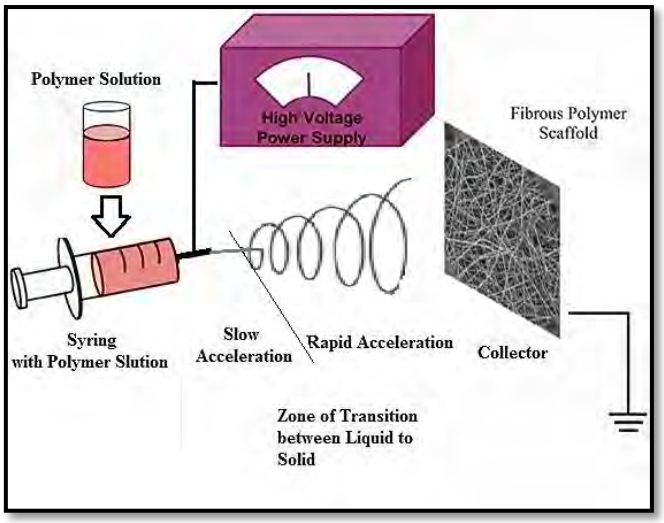
ABSTRACT:

Electrospun chitosan-xanthan gum nanofibers were produced and the correlation between the rheological properties of chitosan-xanthan solutions and electrospinability were investigated at different xanthan gum concentrations. Uniform chitosan-xanthan nanofibers with diameters ranging from 382+182 to 842+296 nm were developed based on the chitosan-xanthan gum content. Overall chitosan-xanthan gum solutions exhibited shear thinning behavior for all the concentrations tested, which tended to increase with the increase of concentration of xanthan. Furthermore the electrical conductivity of the chitosan-xanthan solutions was observed to increase with the increase of xanthan gum concentrations. We can conclude that the optimal electrospinning process is directed by the apparent viscosity properties and the electrical conductivity of the chitosan-xanthan solutions. We are currently investigating the utilisation of these electrospun chitosan-xanthan nanofibers as a carrier for bioactive compounds.



Chitosan/Phospholipids Hybrid Nanofibers and Hydrogels for Life Sciences Applications

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Chitosan(s), a chitin-derived polysaccharides made of glucosamine and N-actetyl glucosamine, exhibit a set of remarkable biological properties such as biocompatibility, biodegradability, hemostatic activity, antibacterial, antimycotic and anticoagulant activity. Subsequently, chitosan (s) have been largely explored to produce nano-micro structures (particles, hydrogels, fibers, films). Likewise, phospholipids, the self-assembling molecular building blocks of cell membranes, constituted by a charged polar head group and a hydrophobic tail that have some biological activities, have been investigated to produce nano-bio structures such as nanoparticles, capsules/liposomes, emulsions and organogels. Therefore, the combination of both chitosan (s) and phospholipids offers possibilities to fabricate structures with suitable biocompatibility to be used within life sciences. This study focused on the development of (i) aqueous stable and biocompatible electrospun chitosan/phospholipid nanofibers [1] and (ii) the preparation of hydrogels by the co-assembly of chitosan and phospholipids [2]. The morphology, water uptake, stability, and biocompatibility of the nanofibers and hydrogels were evaluated using different contents of phospholipids. Moreover, the mucoadhesive properties, encapsulation and *in vitro* release of curcumin, diclofenac and vitamin B12, as model drugs, from the nanofibers was studied, demonstrating their potential as a delivery system for life sciences applications.

Acknowledgments: This work was supported by the European Union funded project “Nano3Bio” (grant agreement no 613931) under FP7.

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Session

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Oral Presentations

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Yeast cell factories for bio-based chemicals

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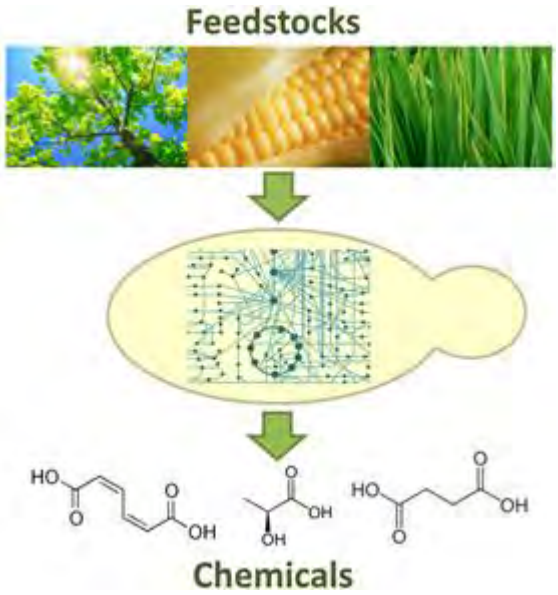
Production of bio-based chemicals requires novel highly efficient and robust cell factories. Yeast makes an excellent host for biorefinery applications and t he recent developments in CRISPR-based technology made genetic engineering of yeast cells cheaper and faster. We have developed an array of CRISPR-based genetic tools that facilitate metabolic engineering of yeast *Saccharomyces cerevisiae*. Using these tools, we have engineered yeast cell factories for production of chemicals, such as 3-hydroxypropionic acid[3], a potential platform chemical for acrylics, and aromatic secondary metabolites with applications as nutraceuticals and cosmetic ingredients (resveratrol[4], *p*-coumaric acid[5], rosmarinic acid, flavonoids).



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Consortia based production of biochemicals.

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One of the great challenges facing society is how to sustainably produce food, chemicals and other commodities required to maintain and develop our current life style. To compete with and ultimately replace existing petrochemical-based manufacturing processes, the development of innovative and effective solutions is needed.

In this project we have explored the possibility of using designed consortiums for the co-valorization of the main carbon sources in lignocellulosic biomass (xylose, glucose, arabinose, and acetic acid). In one study we have used pre-processing simulations, constraint-based modelling, and state-of-the art metabolic engineering tools to develop a consortium of cells capable of efficient valorization of synthetic hemicellulosic hydrolysate. Stable co-existence and effective co-valorization was achieved through niche-differentiation, auxotrophy, and adaptive evolution. In another study, stable consortia based fermentation was achieved through niche partitioning, syntrophy (auxotrophy combined with removal of inhibitory side product), and CRISPRi mediated gene silencing. The achieved results demonstrate that consortium based approaches for valorizing complex biomass and waste related carbon sources can be an attractive alternative to the design of a so-called “superbug” and can thereby add significant value to biorefineries.

Polyhydroxyalkanoates (PHA) production from fermented crude glycerol by mixed microbial cultures.

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Crude glycerol is an abundant by-product from the biodiesel industry, which has recently received much attention as a biorefinery substrate [1]. One of the possible high value products are polyhydroxyalkanoates (PHA), which are biopolymers produced as internal carbon storage in bacteria. These bioplastics have the potential to substitute conventional plastics such as polyethylene and polypropylene, providing that their production cost is lowered [2]. This could be achieved by the use of microbial mixed cultures with no sterilization requirements [3].

Since volatile fatty acids (VFA) are recognized as preferred substrates for PHA production [3], fermented crude glycerol can be used as a substrate. Nevertheless, the anaerobic fermentation of glycerol leads also to significant amounts of 1,3-propanediol (1,3-PDO), a compound which has not been studied as a substrate for PHA production.

The present study included initially a set of enrichment strategies aiming at the production of PHA from all compounds in the fermentation broth (VFA and 1,3-PDO). Although production of PHA from 1,3-PDO was observed to be possible, high yields were not obtained from this substrate. Given that 1,3-PDO is also a high value product, a new enrichment strategy was formulated where only VFA were converted into PHA (up to 70% of the cells dry matter) and 1,3-PDO was recovered from the process (97% recovery). The generated bioplastic was a copolymer of poly(hydroxybutyrate-co-hydroxyvalerate).

Apart from obtaining a stable culture with a high PHA storage capacity, the applied strategy also reaffirmed the possibility of adjusting the metabolic response of mixed microbial cultures by means of the operational conditions of the enrichment. Therefore, a novel biorefinery scheme targeting production of 1,3-PDO and PHA from crude glycerol as feedstock is hereby proposed.

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Session

I

Laptop Presentations

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Session

I

Poster Presentations

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Bio-based chemicals – green, but also sustainable?

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For almost two decades, the chemical industry has put great effort into developing bio-chemicals, among others to fight global warming caused by greenhouse gas emissions, one of the biggest threats that are faced by our society today. To facilitate a growing and versatile bio-based chemical production, the US Department of Energy proposed in 2004 a list of 12 building block chemicals which can either be converged through biological or chemical conversions. Moving toward more bio-based chemicals, the chemical industry does not only claim to reduce climate change impacts, but also that they are increasing overall sustainability in chemical production. Whether such claims are justifiable is unclear. When sustainability of bio-based polymer production is assessed, various environmental trade-offs occur that need to be considered.[1] It is not enough to claim that a bio-chemical is sustainable by exclusively looking at reduced global warming impacts related to avoiding oil refining and related greenhouse gas emissions. However, there is big variation of which impacts are assessed and which life cycle stages are included between existing published studies focusing on assessing environmental sustainability of bio-based polymers.[2]

As an example, when comparing studies focusing on succinic acid, as a final product or building block chemical, bio-based succinic acid (SA) shows a better environmental sustainability performance than fossil-based SA when only “global warming” and “resources depletion” are considered as environmental impacts.[3] When other potentially relevant impacts are included into the assessment, trade-offs become apparent and bio-based SA may show worse environmental sustainability performance for example related to potentially toxic impacts on ecosystems from using pesticides during growing of the organic biomass (feedstock of bio-chemicals), and/or emissions of dust and particulate matter and occupying and using arable land.[4,5]

As the new era in biorefineries is rising, 2nd generation bio-chemicals are based on using waste streams instead of field crops as feedstock. However, it is currently unclear how these systems perform in terms of environmental sustainability related to for example additional energy and materials used during the waste treatment. This requires a full analysis of all relevant environmental impacts to fully support sustainability claims and consistency in environmental assessment studies to be able to identify and address potential hot-spots for reducing environmental impacts in bio-chemical production.

[1] (Weiss et al. 2012)
[2] (Hottle, Bilec, and Landis 2013)
[3] (Cok et al. 2014)
[4] (Smidt et al. 2015)
[5] (Breedveld et al. 2014)

Green Fiber Bottle: the fully biodegradable packaging

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The ambition of the Green Fiber Bottle (GFB) project is to manufacture a fully biodegradable bottle. Carlsberg is the intended end user, and they aim to package their beer in the new bottle. The new product is intended to replace the existing plastic and glass bottles, and thus reducing their impact on the environment, especially the oceans. For example, the life span of a plastic bottle in the ocean is 500 years, and during its degradation, the plastic is reduced to micro pieces, which causes the starvation of several marine animals.

The new bottle is completely made from molded paper pulp, which is a renewable resource. Nevertheless, due to food and drugs limitations, only virgin paper fibers must be employed in the production. The bottle could then be left to biodegrade in nature or enter a recycle system, along with other paper-based product. In order to contain the liquid, the bottle has to have an inner coating barrier. The most reliable solution proposed is to coat the inner walls with silicon dioxide, which is not biodegradable but rather environmentally inert.

To enhance the environmental footprint and sustainability of the bottle, and to be competitive with the existing technologies, the manufacturing technology for the production of the bottle has to offer the possibility of significant energy savings. Molded pulp products are made from wood fibers dispersed in water, and then they are formed, drained and dried. A relatively large quantity of resources (i.e. energy and time) is consumed during the drying process. It is in this process stage that an innovative way of drying the products can be exploited by using the concept of impulse drying. Impulse drying is an advance drying technique in which water is removed from a wet paper pulp by the combination of mechanical pressure and intense heat. In this process, the wet pulp is exposed to pressures ranging from 30 bar to 50 bar and temperatures typically between 200 °C and 400 °C. At these intense conditions, the wet pulp is dried in the order of seconds.

Many challenges must be dealt with to enable the use of such improvement in the production of the GFB. One of the research topics currently under investigation is the understanding and modelling of the impulse drying effect. Experimental evidence proves that a part of the liquid content in the paper pulp transforms into steam, and the correlated expansion eases the movement of the water out of the product. This secondary effect should be at the base of the reason why the drying takes place in a considerable short time. Nevertheless, a complete understanding of the phenomena has not been achieved, and thus a complete control of the drying mechanism is yet to be realized. The need of a physical model is thus clear in order to enable the use of impulse drying in a production environment.

Biodiesel from microalgae – greenhouse gas emissions and energy balance

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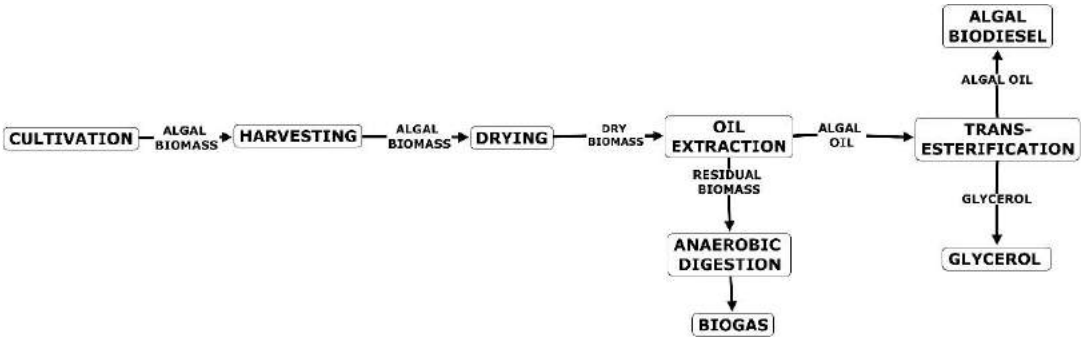
The current use of fossil fuels is problematic for both environmental and economic reasons and biofuels are regarded as a potential solution to current energy issues. This study analyzes the energy balances and greenhouse gas emissions of 24 different technology scenarios for the production of algal biodiesel from Nannochloropsis cultivated at industrial scale in photobioreactors in Denmark. Both consolidated and pioneering technologies are analyzed focusing on strengths and weaknesses which influence the performance. Based on literature data, energy balance and greenhouse gas emissions are determined in a comparative 'well-to-tank' Life Cycle Assessment against fossil diesel. Use of by-products from biodiesel production such as glycerol obtained from transesterification and anaerobic digestion of residual biomass are included. Different technologies and methods are considered in cultivation stage (freshwater vs. wastewater; synthetic CO2 vs. waste CO2), harvesting stage (flocculation vs. centrifugation) and oil extraction stage (hexane extraction vs. supercritical CO2 extraction). The choices affecting environmental performance of the scenarios are evaluated. Results show that algal biodiesel produced through current conventional technologies has higher energy demand and greenhouse gas emissions than fossil diesel. However, greenhouse gas emissions of algal biodiesel can be significantly reduced through the use of 'waste' flows (nutrients and CO2) but there are still technical difficulties with both microalgae cultivation in wastewater as well as transportation and injection of waste CO2. In any way, a positive energy balance is still far from being achieved. Considerable improvements must be made to develop an environmentally beneficial microalgae biodiesel production on an industrial scale. In particular, different aspects of cultivation need to be enhanced, such as the use of wastewater and CO2–rich flue gas from industrial power plants.



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Laccase-3D graphene as catalysts for oxygen reduction in biocathodes

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Biofuel cells are devices that transform chemical energy to electrical energy using enzymes as catalysts to oxidize fuel molecules, rather than precious metals. Laccase is a blue multicopper oxidase with selective catalysis for O_2 reduction to H_2O at low overpotential [1]. Therefore, the use of laccase as a biocatalyst for developing biocathodes in enzymatic fuel cells is feasible and interesting.

Graphene, a two-dimensional (2D) crystal carbon sheet, has received much attention since its discovery because of the unique electronic properties [2,3]. 3D graphene exhibits improved performances with respect to 2D graphene materials, because of their large accessible specific surface areas, interconnected conductive network, and special microenvironment [4].

Novel type of 3D graphene electrodes are expected to immobilize laccase for developing biocathodes. The aim is an efficient direct electron transfer (DET) enzymatic electrode with a high coverage of active biocatalyst molecules on the electrode and fast electron transfer between the redox sites of the immobilized enzyme molecules and the electrode surface. Schematic idea is presented in Figure 1.

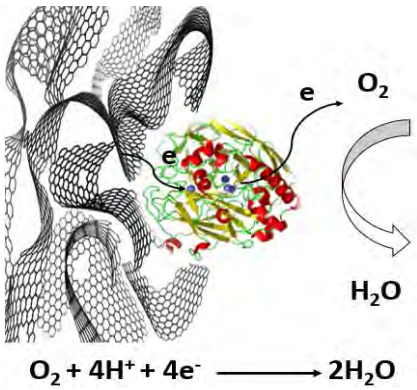

Fig. 1 Immobilization of laccase on 3D graphene for construction of biocatalysts.

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Session

L

Oral Presentations

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Smart-Energy Operating-System - A Framework for Implementing Flexible Electric Energy Systems in Smart Cities

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The ***Smart-Energy Operating-System (SE-OS)*** framework has been developed within the CITIES research project (www.smart-cities-centre.org). This framework enables a systematic approach for implementing flexible electric energy systems in smart cities. The SE-OS methodologies are based on methods for data analytics, cyber physical modelling, forecasting, control, optimization, IoT, IoS, and cloud computing. The SE-OS concept has being used for enabling flexibility and demand response in smart cities in a large number of demo project. Finally it is shown that SE-OS in combination with methods for energy systems (gas, thermal, power, biomass, fuel) integration can provide virtual energy storage solutions on all relevant time scales, ie. from minutes to seasonal storage.

The ***Smart-Energy Operating-System (SE-OS)*** is used to develop, implement and test of solutions (layers: data, models, optimization, control, communication) for ***operating flexible electrical energy systems*** at **all scales.**

Living Labs – From scientific labs to the smart city

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Research laboratories are characterized by the fact that the experiments are carried out under very well controlled conditions. In some research fields, field trials are a well-established methodology where many of the parameters involved are not controlled by the researchers in their experiments. Living Labs can be compared with these field tests, trails and setups. However control of parameters is often not possible in living lab trials and experiments. Data collection is one of the important subjects and tasks in such research. Often, the researchers and research communities are part of these living labs. Hereby the scientific approach has to be carefully evaluated and methods adjusted accordingly.

Examples of living labs can be found across DTU. A very small living lab is made at the Library where a lighting system is established that can be influenced by students and researches through open interfaces. The basic idea is to enable innovators to perform their developments and research in this real world setup and learn to define solutions that are applicable there.

On a larger scale, DTU is promoting the whole campus as a living lab that can be used for research and development by its employees, but also partners from outside. This proposition can be found under the term “Smart Campus” with it’s own homepage. Here you find the example from the library above, the Smart Avenue that enables communication and IT solutions on the campus, enabled through intelligent street lightning that in the same time is part of the Doll Living Lab setup placed in the area.

Lyngby Smart City is a living lab approach facilitated by the City of Knowledge. Together with the labs presented above, we find a direct chain from scientific research labs at DTU over the campus lab, out into the real world living labs near Lyngby and from there into the big smart city of Copenhagen to be promoted to the world markets. This way the value chain “from research to invoice” is instantiated into not only an innovation and business strategy, but rather a research strategy that aims at elevating DTU’s research to an even more leading international position.

Can we create a whole new urban water system with much higher efficiency and sustainability?

Henrik Kærgaard, Director Cross-Cutting Development, NIRAS, hka@niras.dk

There are strong indications that the future people in the world will to a still larger extent live in the cities and urban areas, so it becomes more and more important for the overall sustainability of the planet to make the cities of the world sustainable. This is an enormous challenge, but also a rather specific and concrete one – and existing and future technology will play a crucial role here.

So what are the actual and potential problems and the future technology outlook of the water sector? In this brief characterization of the history, present conditions and future potentials of the water and utility industry, we argue that the future potentials for further development, innovation, efficiency and customer adoration in the industry are virtually unlimited and basically not constrained by lack of new and relevant technology or funds for investments. The only real limitations are inside our own heads and minds – and what we need to get things moving forward is basically:

- Strong and visionary leadership from the leading stakeholders in the industry
- Strong legal and financial incentives to move towards more sustainable and productive goals, and
- New ways of cooperation, unifying the efforts from the main stakeholders like knowledge sectors, utility companies, component suppliers, public administrations, politicians etc.

Some questions that we pose and try to provide some answers to in this presentation:

- Can we cut water consumption in urban water systems by 90% by changing our ideas of water installations and use in housing and industry?
- Can we make a future urban water system without waste water production? – and consequently without purification plants?
- …and instead produce a large volume of raw materials for the future urban energy production – i. e. not waste but a valuable resource?
- Can we provide a much more attractive service to our citizens than we do today?

We believe that all this is possible – and moreover that it can be done to a very large degree based on existing technologies and products on the global market. However it is of course important, that these technologies and products are combined and used together in new combinations in urban areas – and it is also important to realize that the necessary changes in existing urban areas have to take place over several decades and in a close cooperation and coordination between stakeholders that generally do not cooperate to day. That means comprehensive long term planning in new and more complicated settings, than we are used to – on other words a profound change in our organizational thinking and general mind-set.

In other words a very groundbreaking and demanding innovation challenge – but with a massive potential!

EnergyLab Nordhavn – Progress and Physical Implementation

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EnergyLab Nordhavn is a large-scale integrated research and demonstration project that contributes to the grand challenge of transforming the energy system to efficiently integrate a large share of renewable energy. The project focuses on a cost-effective future smart energy system that integrates multiple energy infrastructures (electricity, thermal, transportation) and provides an intelligent control of subsystems and components – providing necessary flexibility for efficient utilisation of renewable energy. The project results will be based on combining a number of elements established or under establishment in Copenhagen's Nordhavn, one of the largest development districts in Europe.

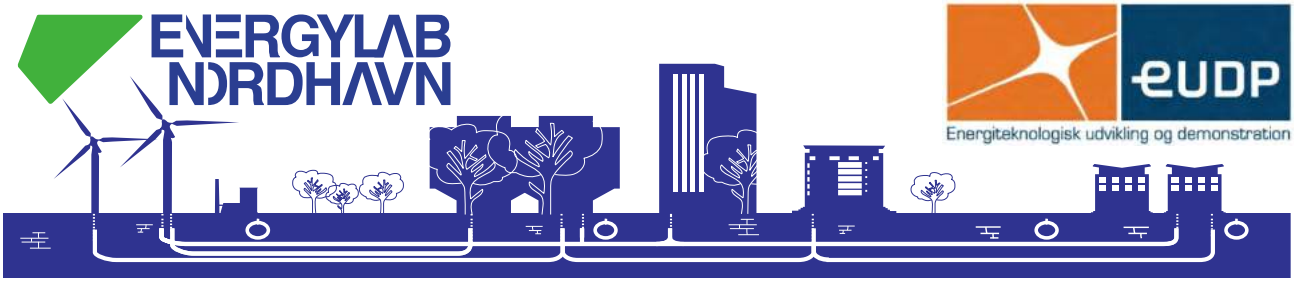
With a diverse set of such elements in the electrical and heating grids, in the built environment, and involving citizens in the area, the EnergyLab Nordhavn project is well on the way to establish itself as a living laboratory and an environment for strong research-based innovation in smart energy technologies, innovative business models and energy management tools for the future sustainable low-energy city districts.

Particularly exciting is the synergy between

- the physical density of the environment in Nordhavn
- the "settler attitude" of the new local population
- new trends of co-creation and participation.
- new tools creating awareness on carbon footprint and other environmental impact.

EnergyLab Nordhavn partners are DTU BYG, DTU MEK, DTU CEE, Københavns Kommune, DONG Energy Electricity Distributions, HOFOR, By&Havn, ABB, Danfoss, Balslev, MetroTherm, Glen Dimplex, CleanCharge and the PowerLab facilities.

The project has a total budget of € 19 mio, of which € 11 mio are funded in two rounds by the Danish Energy Technology Development and Demonstration Programme (EUDP).



Session

L

Laptop Presentations

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Smart Campus and Smart Transport

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During the last 5 years there has been teaching in sustainability at Ballerup campus in different contexts. Based on these experiences the project Sustainable Production was formulated in 2014 and obtained funding from "Industriens fond" for 2015-2017. The presentation will present some innovation ideas created in this project as part of a work package highly focused on tools.

As stated in Ref. 1 "More than three-quarters of total inland freight transport is carried out on the road — slightly more than in 2000". This large transportation industry holds many sustainability issues. The CO2 emission from transport on the road is the biggest contributor to greenhouse gas emissions as shown in figure 1. One way to reduce the emission is through Smart Transport which includes many different disciplines. Here we zoom in on a few of them.

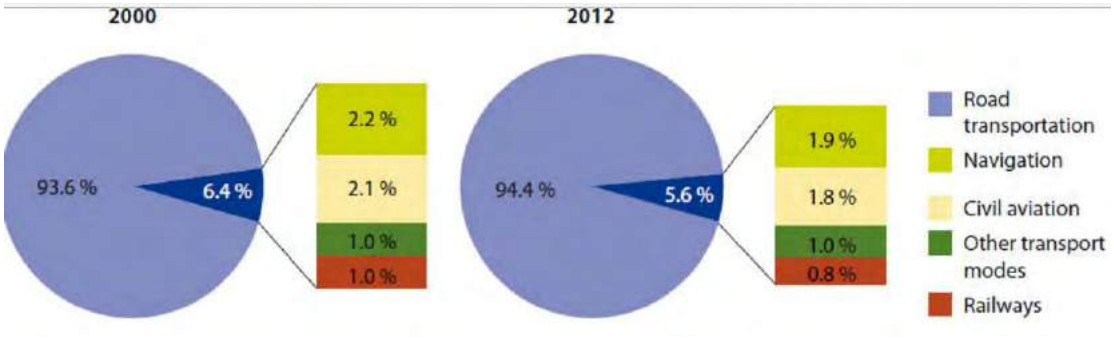

Figure 1: Greenhouse gas emissions by economic activity, EU-28, 2008 and 2013 (1)
(% of total emissions in CO_2 equivalents)

One discipline within Smart Transport is efficient driving where fewer stops and queues would save fuel consumption, emissions and also reduce wear on roads. In this presentation we will mention results from an elective course, where students have worked on a project with focus on creating an application to help the driver of electrical vehicles optimize the route. The work within route optimization, where the driver is guided about the best route based on historical, present and real-time traffic data of different origin is continuing with a demonstrator as outcome next year. Another Smart Transport discipline is efficient parking. At the moment we are building on Ballerup campus parking lot a smart parking monitoring system based on the principles from the Smart Allè at Lyngby campus.

To reduce emissions we need data and the ability to analyze and learn from Big Data. At Campus Ballerup we have started collecting and creating Smart Campus Big Data. The idea is to integrate data such as indoor climate (temperature, humidity, CO2 and noise), and electrical energy consumption as well as district heating and water. The vision is that the industry can see how data can support the decisions for saving energy and water by sampling data from enough sensors locally monitoring energy and indoor climate. One example for perspective is how electrical fingerprints can be used to predict when a machine should be maintained. We will present some data from the current stage of the data-platform progressing towards another demonstrator next year.

The presentation will present student's projects done, ideas/visions for projects using the Smart campus data

Ref1: http://ec.europa.eu/eurostat/statistics-explained/index.php/Sustainable_development_-_transport 7-11-2016

Session

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Poster Presentations

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Local sensitivity analysis for radiant floor cooling system for energy efficiency and thermal comfort

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Introduction

Pre-cooling radiant floor systems takes advantage of using less expensive electricity prices and cooler outside conditions during the night and early morning. Often this allows the use of cooling towers instead of chillers. The objectives of this research are to demonstrate the possibility of using pre-cooling floor slab as an energy efficient cooling system and finding an energy efficient cooling floor slab with appropriate properties. It can be challenging to find the optimal control option for a HVAC system or determining which properties affect the removal of loads in a zone, by experiment. Using simulation software is the best tool to exploring the proper system and building physics. We used IDA ICE to simulate the operation of a cooled radiant floor system. IDA Indoor Climate and Energy (IDA ICE) is a building performance simulation tool that can be used to study the indoor environment in buildings as well as determining the total energy consumption and surface temperatures of the buildings.

Methods

The model was calibrated using data collected at the LBNL FLEXLAB facility. Several simulations in different climates were examined to compare and find the slab properties and control strategy that yielded the highest energy performance. The system used a radiant cooled floor to remove the majority of the cooling load, though there was also a ventilation system. We evaluated several water supply temperatures to observe the difference in the floor surface temperatures and floor surface heat gains. We examined an appropriate nighttime pre-cooling strategy in different climates to keep the building cold during the day time while solar heat gain added to other internal heat gains. Operative temperature and floor surface temperature are the main factors that can illustrate how water supply temperatures affected heat transfer. The paper compares performance of the hydronic system under different control systems floor slab properties and climates.

Results

The simulated model was accurate and the results in main parts verified. The night time pre-cooling control strategy had a significant effect on energy efficiency compared to the day time control strategy. The results showed that slab properties (for example; material and depth of the embedded pipe in the concrete) had a significant effect on energy efficiency and comfort, while water supply temperature in the hydronic system had less of an effect.

Conclusion

Night-time pre-cooling combined with an appropriate air system was more energy efficient than controlling the radiant system during the day; while this system could meet the category 2 standard EN-15251 for occupant comfort.

Successful Implementation of Energy Strategies in Local Communities through Strategic Navigation between Professions

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Implementing sustainable energy strategies in local community development projects is far from straightforward, which can be seen by reference to the common 'implementation gap' that can be observed if energy strategies get compared to implementation rates of renewable energies in reality. Such an implementation process can be categorized as a 'wicked problem', to which definitive and objective answers do not exist[1]. Rather, a diversity of goals are being politically pursued as a result of a prevailing plurality of publics, making the act of planning sustainable cities a difficult challenge for the professionals involved.

The work in the IEA EBC Annex 63[2] provided the basis to collect narratives about successful implementation of energy strategies in local community development projects in more than ten countries. In studying the front runner case studies we were able to find first indications of a pattern on how planners navigate in this complex setting of interests with the planning tools and approaches that they have at hand. This is carried out through analyses of how champions in different cities have succeeded in implementing certain energy strategies in specific local communities.

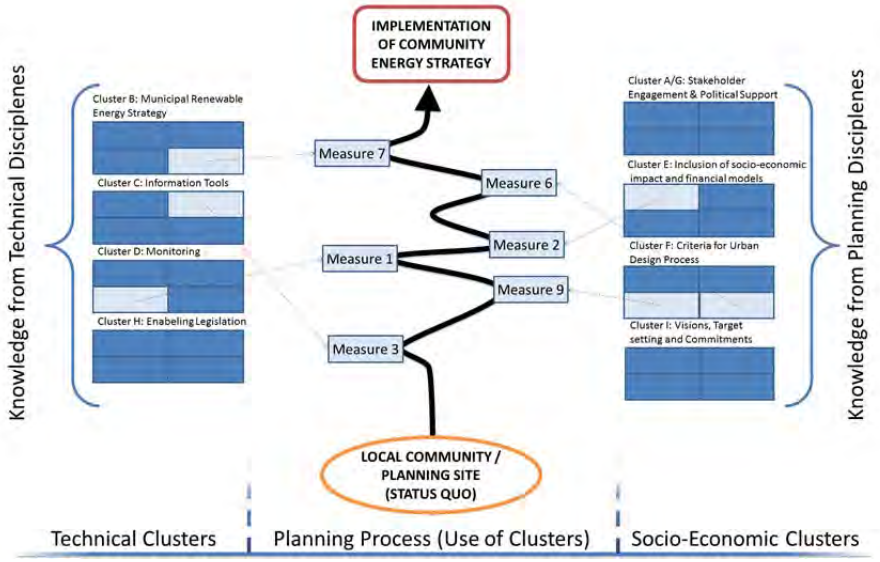

Figure 1: Model of an implementation process, using different knowledge sets & planning tools

The interaction between the professional fields of urban and energy planning, respectively, is crucial for implementing energy strategies locally. First findings from our case studies are that the interaction between these two professions occurs in a much broader context of different communities of practice, involving other stakeholders like politicians, developers, end-users and the like. In the selected case studies, we can see that planners deliberately seek to extend traditional planning approaches, like e.g. regulation, with broader context-specific learning processes. In doing so, we argue that – what we call – an implementation synergy is established by interlacing different forms of situational knowledge with strategic knowledge about how to reach a desired energy target (see figure 1). As one outcome it is possible identify different domains of knowledge that can be exploited strategically in order to create an implementation synergy in local development projects. This understanding could contribute to tame the 'wicked problem' of implementing energy strategies in local communities.

1 Rittel, H.W.J. & Webber, M.M. Policy Sci (1973) 4: 155. doi:10.1007/BF01405730
2 http://www.annex63.org/

Impact of Prosumer Buildings and their Clusters on the Energy System – project outline

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With the global and national policies for the reduction of greenhouse gas emission, increasing capacities of renewable sources are being installed. As those are becoming profitable, small actors in the market are becoming more important, changing the paradigm of the centralized, top-down operation [1] and calling for new business models and operation logic appropriate for prosumers [2, 3].

Prosuming buildings produce and consume energy, typically renewable energy from photovoltaics, solar heat and wind, but may also store energy by local means.

The study aims at investigating the implications of being prosumer and the consequences it has on the common energy system, for all energy carriers, gas, electricity, heating and cooling, both for individual and for collective prosumers. [4] We hypothesize that the interaction of a growing number of prosuming buildings using mainly renewable energy sources with the energy system can be improved by smart integration and optimized operation schemes.

This research in its initial stage is hosted by the Section for Building Energy at the Department of Civil Engineering, as part of the participation in the strategic research centre project CITIES, specifically Work Package 3 on “Intelligent Energy System Integration” [DTU Civil Engineering]. The project is carried out in cooperation with CITIES Work Package 2 on “Energy Supply, Transmission and Conversion" [DTU Energy Conversion]. [4]

The purpose of the study is to find an optimal operation strategy for prosuming buildings. The single user definition is expanded to include collective prosumers where neighbourhoods, districts or whole cities go together to produce their energy. Different types of prosumers will be identified and grouped based on data, taking part in different parts of the energy system (including, but not limited to rooftop PV in the electric network as well as prosumers in district heating).

References

[1] D. J. Vergados, et. al, “Prosumer clustering into virtual microgrids for cost reduction in renewable energy trading markets,” *Sustain. Energy, Grids Networks*, vol. 7, pp. 90–103, 2016.

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[3] J. Rodríguez-Molina, et. al, “Business models in the smart grid: Challenges, opportunities and proposals for prosumer profitability,” *Energies*, 2014.

[4] "PhD scholarship in CITIES for IT-Intelligent Energy Systems for Cities” http://www.dtu.dk/, 2016

Dynamic optimization of building performance: Use of real-time building data for improving facilities management

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In this digital age many companies consider data as new oil. It also includes facilities management organizations. Facilities managers in many private and public organizations are interested in data sets on building characteristics, operation and maintenance activities, usage patterns, space management, energy management, asset management etc.

The research focus of this industrial PhD is to study how these different building data sets can be used and combined for improving total value of buildings, with special emphasis on environmental building performance from lifecycle perspective.

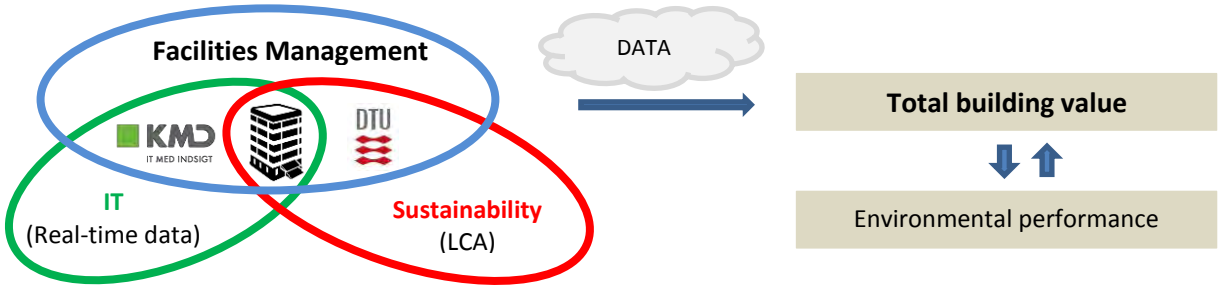

Figure 1: Project design and research focus

The project follows the implementation of Integrated Facilities Management System *KMD Atrium* in Danish Facilities Management organizations. The focus is on non-residential buildings from user- and facilities manager perspective. By studying the implementation effects of KMD Atrium, this industrial PhD develops a methodological basis and purpose-based software for simultaneous calculation of total value and environmental performance of non-residential buildings.

So far, a literature study has identified 8 indicator categories that should be considered when addressing environmental performance of building: Energy, GHG emissions, Water, Waste management, Land use, Building materials, Reuse/recycling potential and Indoor Environmental Quality. The study indicates that research is mainly focusing on energy and GHG emission related topics, while other environmental categories are not investigated sufficiently.

The next step of the project combines research and practice through various case studies in which environmental building performance of non-residential buildings will be studied. Case studies will investigate which environmental indicators are used in practice and why, and disclose how building data related to these indicators is collected, used and combined.

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Session

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Oral Presentations

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Advanced microstructural analysis of cyclically deforming metallic materials towards lifetime improvement

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Periodically repeated loading of metallic components can result in unexpected catastrophic materials failure limiting the component lifetime. As manufacturing of metallic components in general is energy and combustion intensive, an increased performance will lead to a more efficient use of resources and limit the environmental and economic impact from production. Furthermore, the enormous exchange and transfer costs of large components that fail due to cyclic deformation can be reduced with optimized material selection and design.

The presented investigations should form a basis for future developments in the lifetime assessment of metallic materials. As any material inherits its mechanical properties from its internal structure, structural investigations on a submicroscopic level are needed. For an understanding of the structural development during cyclic deformation before fracture, the microstructure on an aluminium alloy AA1050 was characterized in detail by advanced electron microscopy (EBSD, cf. Fig. 1). Additionally, high resolution reciprocal space mapping was performed successfully for the first time during cyclic deformation experiments *in-situ* on bulk samples at Argonne Photon Source. While monitoring macroscopic stresses and strains during several load cycles, diffraction peaks of single grains were monitored. Due to the characteristic intensity distribution for ordered defect structures, elastic strains of single grains as well as their individual subgrains can be resolved. Both, grains and subgrains were followed during individual load cycles (cf. Fig. 2). Individual radial profiles were analyzed showing that the peak position during a load cycle follows the hysteresis. With the present technique, it is possible to relate internal stresses in a new way to the macroscopic deformation of the sample. This will allow improvement and further establishment of multiscale models for a better prediction of the materials and component lifetime.

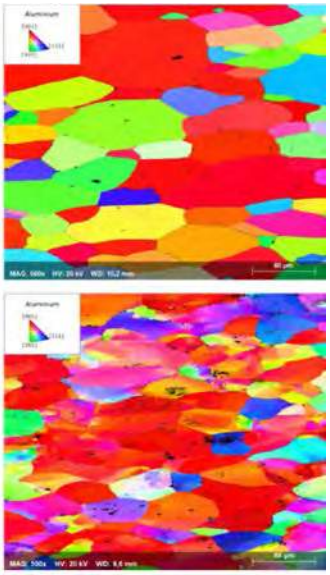

Figure 1: Orientation maps before and after cycling for 5000 cycles obtained by ESBD showing developing subgrain structures

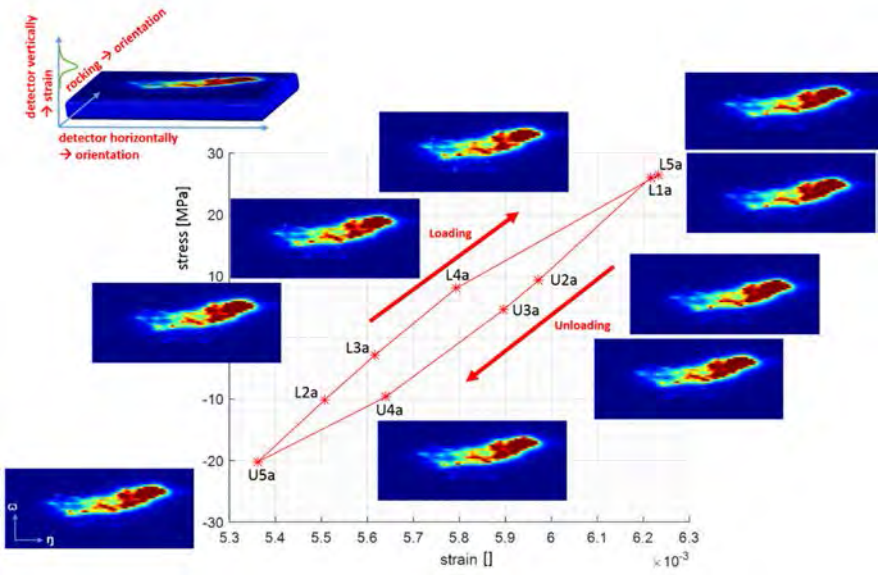

Figure 2: Azimuthal maps acquired during a single tension-compression load cycle at APS 1-ID-E using High Resolution Reciprocal Space Mapping. Azimuthal maps are projections of the intensity distribution along the scattering vector representing the internal structure and orientation distribution within individual grains.

Strong and light-weight materials made of reinforced honeycomb sandwich structures

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In the transport sector, new strong and light-weight materials can reduce the weight of airplanes, cars and containers. This will lead to a reduction in CO_2-emissions as less weight needs to be transported.

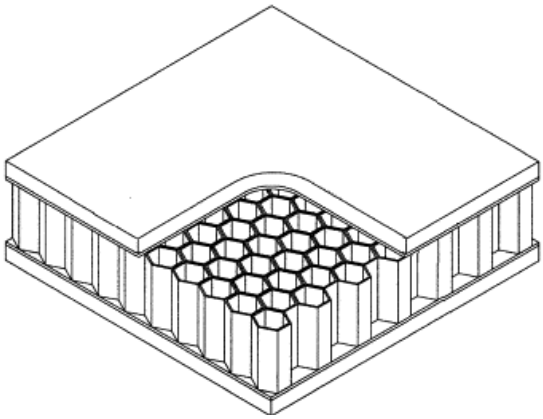

Figure 1: Sandwich material

The requirements for these light-weight materials are that they need to be strong and have a low cost, in order for them to compete with conventionally used materials like steel or aluminum.

A great candidate for a material that can fulfil these requirements of being light, strong and low cost is a sandwich material. A sandwich material is a material that is made of a light-weight core with a thin layer of steel or fibre composite on top and bottom of the core.

The core in a sandwich material is typically made of a honeycomb structure. Honeycomb structures have been used for more than 50 years. Until now honeycombs have been expensive to produce. However, with a new production method it is now possible to produce honeycombs structures at a low cost.

Figure 2: New production method

In a large collaborative European project called INCOM, the possibility of reinforcing the honeycomb structure is investigated. The honeycomb structure is reinforced with sustainable fibres as the fibres are extracted from saw dust.

Application of powder X-ray diffraction in materials science

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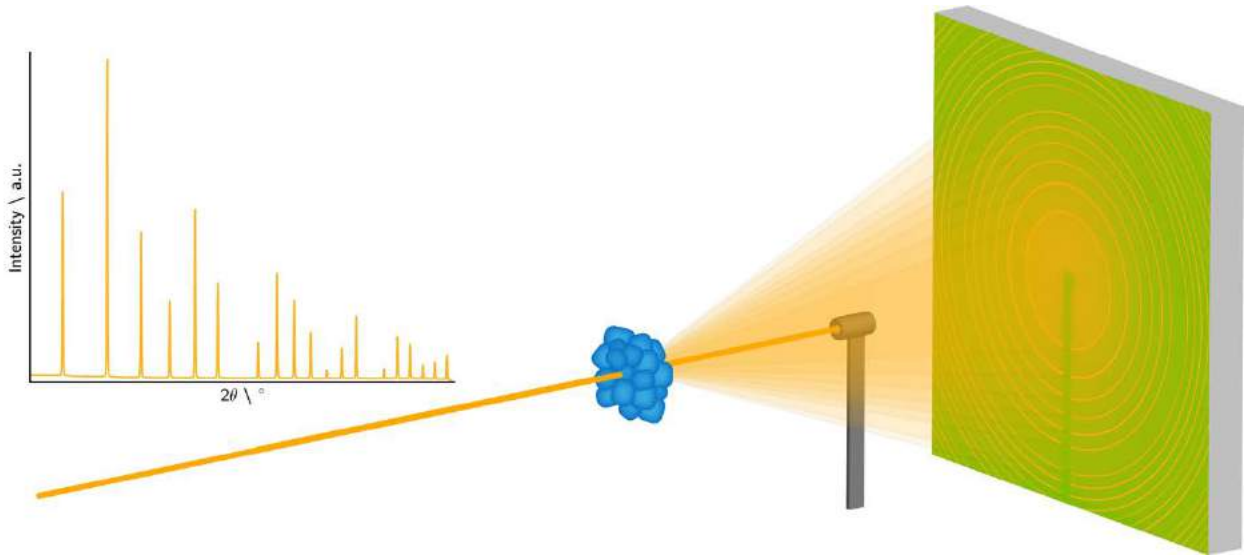
The powder X-ray diffraction (PXRD) technique has been around for a century and is today one of the most powerful ways to study the atomic structure of microcrystalline materials. The technique was for a long time used mainly for phase identification, but is today an invaluable tool for researchers and industry in many different fields. This development is largely caused technological developments in e.g. X-ray sources and detectors, and exponential increase in computing power. Especially the availability of extremely bright X-ray beams from modern synchrotron facilities have advanced the field.

The high intensity and fast detectors are being utilized together with creative sample environments to emulate material performance under working conditions in real time. The Danish PXRD and X-ray Imaging communities have joined forces and are currently building a unique instrumental platform, DanMAX. DanMAX will perform experiments ranging from classic PXRD, through PXRD/Imaging hybrid experiments, to classic Imaging. The beamline will be built at the new MAX IV synchrotron in Lund Sweden and is expected to be operational in 2019.

In my presentation I will give an introduction to the technique and present the visions for the new Danish beamline, DanMAX. In addition, I will present a number of applications examples from out lab where PXRD has been used for characterization of energy materials.



Quantifying the onset of recrystallization in deformed metals using x-rays

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Understanding the internal structural dynamics of metals during annealing is crucial for their use and manufacture. The role and dynamics of subgrains and newly formed recrystallizing grains are important to annealing, but are largely unknown due to the lack of appropriate techniques for mapping their shape, orientation and distribution *in situ*.

Here, we present an annealing study in which the subgrain sizes and orientations inside a cold-rolled and partly recrystallized specimen of aluminium were monitored with high angular resolution during heating. Hard x-rays were diffracted from the polycrystalline sample onto a high resolution detector and the sample was tilted in small steps to map a section of orientation space, see Fig. 1. More than 10^3 subgrains of equivalent radius of 1-2 µm was identified and characterized to show the evolution of the size-distribution with temperature. We demonstrate how individual subgrains and subgrain structures may be tracked as they evolve during the recovery and recrystallization processes.

Furthermore, we map the intragranular structure of newly formed recrystallizing grains of ~20 µm radius by means of a recently developed technique, dark field x-ray microscopy, in the diffracted x-rays are selected and magnified to give real space images of the spatial distribution of a particular lattice orientation. With angular resolution of mrads and spatial resolution of 100 nm we map orientation distributions and mosaicity from a series of images obtained at slightly different tilt in two perpendicular directions, see Fig. 2. From these maps we quantify the structural changes upon further annealing.

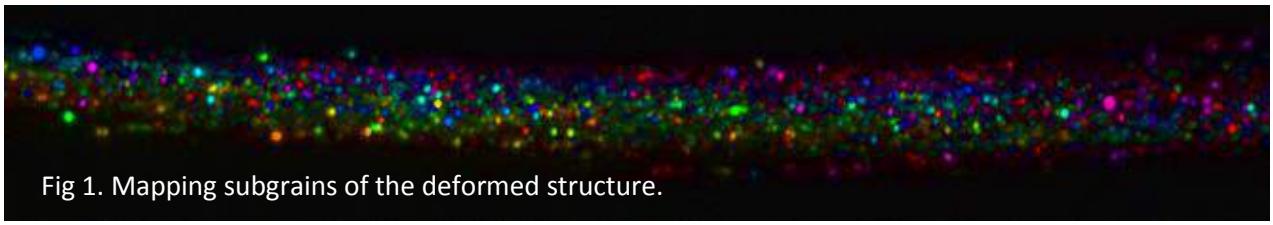

Fig 1. Mapping subgrains of the deformed structure.

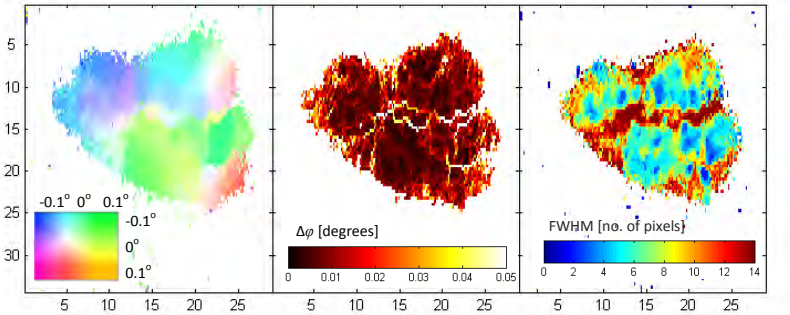

Fig 2. Mapping a recrystallizing grain.

2D materials as protective coatings

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The economical losses related to corrosion represent 3-4 percent of the world's gross domestic product [1], and the load on environment as well as damage and accidents due to waste products and mechanical failures are very serious as well. Corrosion protection of metals is often done by coatings, and the discovery that graphene - a mono atomic layer of carbon atoms - is impermeable and chemically inert, have led to research in its relevance as a barrier coating [2]. It was soon pointed out that galvanic corrosion can lead to acceleration of corrosion of a metal in contact with graphene in an ionic medium, in the case that a tear or hole in the graphene, as the graphene is more noble than any metal [3]. We have studied different possible approaches to counteract this problem: one is to grow thicker films, and thereby reduce the chance of macroscopic damage. This can be done by chemical vapour deposition on electroplated nickel, which can be done on many metal and alloy surface. The performance of the multilayer graphene coatings are excellent in saline environments, however, hydrogen evolution at the interface cause bubble formation and delamination in acidic solutions. A different approach is to replace the conductive graphene with another 2D material, hexagonal boron nitride, an electrical insulator with atomic structure properties very similar to graphene. We studied the protection against oxidation by both single layer graphene and single layer boron nitride, both grown by chemical vapour deposition, and find that the long-term resistance to oxidation is far better for hexagonal boron nitride. We compare the pros and cons of the different approaches for realistic applications.

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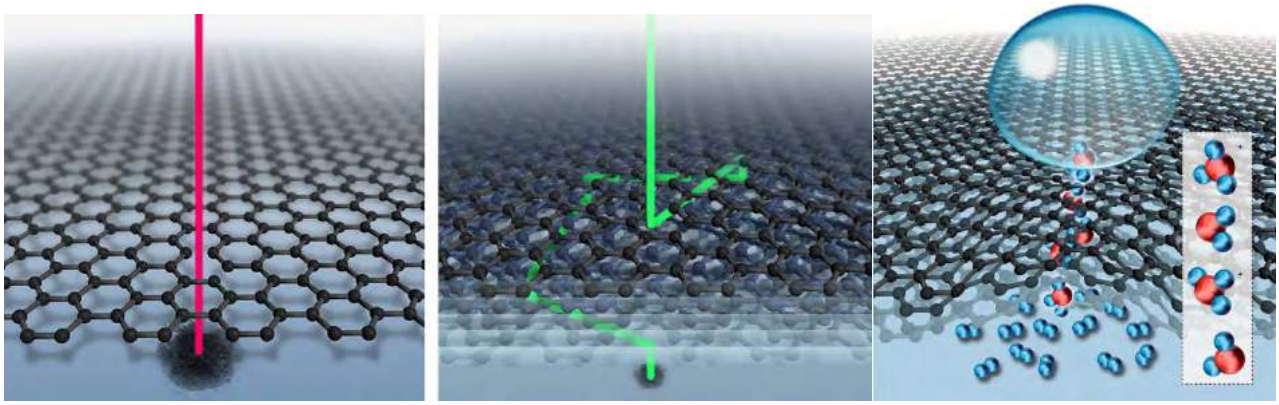

Coatings for High Temperature Corrosion Protection of Stainless Steels

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The application of stainless steels in important high temperature technologies such as solid oxide cells (SOC) is limited by corrosion. At the typical SOC operating temperature (> 650 °C) rapid growth of a poorly conductive oxide scale leads to increased resistance across the SOC stack with time. Furthermore, the oxide scale is prone to form volatile Cr(VI) species that have been shown to degrade the performance of the SOC oxygen electrode. One way to mitigate these issues, and thereby increase the lifetime of the stainless steel component, is by use of protective coatings.

At DTU Energy we are working on development and evaluation of various protective coating materials such as $(Mn,Co)_3O_4$, Y_2O_3, CeO_2 and Al_2O_3. The choice of coating material is tailored to the exposure conditions and requirements of the specific application. An example of the effect of a protective coating intended for the air side of interconnects in SOC stacks is shown in Figure 1. By coating Crofer 22 APU with $MnCo_2O_4$ the oxide scale thickness formed after 2000 h at 900 °C was reduced by a factor of five. The coatings are typically applied to stainless steel by electrophoretic or electrochemical deposition, which allow careful control of the coating layer thickness. Oxidation testing is performed under realistic conditions in various atmospheres and the corrosion behavior is characterized by thermogravimetric analysis and measurement of area specific resistance. X-ray diffractometry and electron microscopy is used for post-mortem analysis of tested samples. An overview of these activities at the DTU Energy and some highlights of the latest results will be presented.

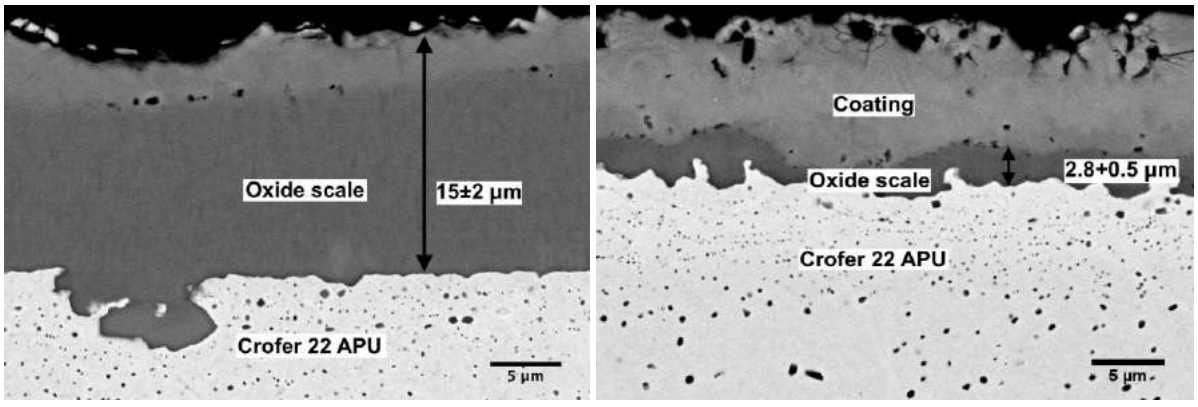

Figure 1: SEM cross sectional micrographs of samples oxidized 2000 h at 900 °C in air. Left: uncoated Crofer 22 APU alloy. Right: Crofer 22 APU coated with $MnCo_2O_4$.

Shaping our energy future by electrospinning

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Electrospinning is the most versatile technique to design nanofiber materials with numerous applications in the fields of filtration, membranes, catalysts, reinforcement and biomedicals. Using electrospinning, we are able to design a complex structure from a rich variety of materials including polymers, metals, ceramics and composite, with the ability to control composition, morphology and secondary structure and tailor performance and functionality for specific applications. Moreover, with significant improvement in electrospinning equipment design, industrial-scale electrospinning technologies with production rate of several thousands of square meters per day are transforming advanced material research done in our labs into products serving our everyday life.

This talk will show you the power of electrospinning technology with exciting projects that address the sizable challenges in energy devices by electrospinning. The outcomes of these unique nanofibirous structures are significant improvements in electrochemical performance and durability, which bring our sustainable energy technology one step forward.

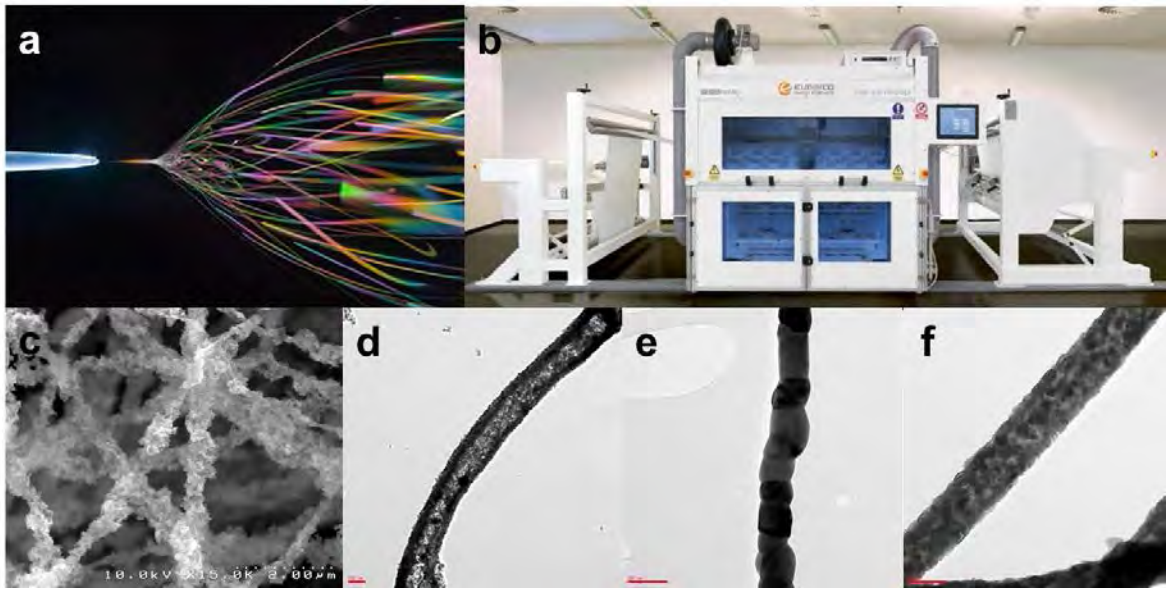

Figure 1. a) Electrospinning process; b) Industrial-scale electrospinning equipment (Elmarco); c) Pt-C/Nafion nanofiber electrodes for PEMFCs; d) metal oxide nanotubes; e) metal oxide nano-pearl string; f) metal oxide nanofiber.

Non-destructive integration of graphene for organic light emitting devices

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The number of smartphone users worldwide is expected to grow above 2 billion during 2016 and approach 3 billion by 2020 [1]. An increase in production of touch screens is required to follow the demand and similar increasing demands for optoelectronic devices such as solar cells and (organic) light emitting diodes (OLED/LED) exist. A standard component in this class of devices is the transparent conducting electrode; a layer of material functioning as contact on one side of a device while simultaneously allowing passage of light. The current industry standard for the transparent conducting electrodes is indium tin oxide (ITO) which has a low sheet resistance and high transparency. Drawbacks of ITO include the high cost of indium as a raw material and process restraints, which makes this oxide system less attractive for low cost and high volume applications [2]. This means that the search for possible ITO replacements is ongoing.

Atomically thin carbons films known as graphene were first isolated in 2004 [3] and have since been the subject of extensive research due to its list of extraordinary properties including being the strongest compound discovered, high transparency, efficient conductor of heat and electricity, and being flexible/foldable [4]. The set of properties that graphene can offer is ideal as ITO replacement for optoelectronic devices and could lead to a new class of flexible electronics including solar cells that can be easily placed on uneven surfaces. Large area production of graphene is based on chemical vapor deposition, where a copper catalyst is heated to approximately 1000 °C in the presence of carbon containing precursors. In order to integrate graphene into a working device, it must be transferred from the copper catalyst, which conventionally is done by etching the copper support leading to unnecessary waste of copper while generating harmful chemical waste.

We develop sustainable, efficient ways to grow, transfer and characterize graphene with a minimum of resources: growth on reusable copper substrates, non-destructive transfer by oxidative delamination and fast, non-contact electrical characterisation using terahertz time-domain spectroscopy. In the talk I will present recent results demonstrating that the material consumption can be reduced dramatically by using non-destructive processes to produce transparent electrodes for OLEDs, but also discuss some of the technological bottlenecks and challenges yet to be addressed.

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Session

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Laptop Presentations

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Bi-metallic nanoparticles for optical hydrogen sensors

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The recent market introduction of fuel cell cars has increased the interest in safe and accurate hydrogen sensors for mobile applications. We explore supported arrays of bi-metallic nanoparticles as transducing elements for optics-based hydrogen sensors. In particular, Pd-Au nanodisks are very promising since they provide a linear, hysteresis-free response to hydrogen absorption and desorption [1,2]. We employ advanced electron microscopy characterization to investigate the correlation between the structure at the micro-and nanoscale with the macroscopic properties of the nanoparticles, and to understand the improvement of performance observed for Pd-Au as compared to pure Pd sensors.

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Effect of substrate curvature on Mn-Co-O spinel coatings prepared by electrophoretic deposition for solid oxide fuel cells

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Solid oxide fuel cell technology enables efficient and clean conversion of chemical energy (hydrogen containing fuel) into electrical energy and heat, with very low emission of NO_x and CO_2 gases. Most recent fuel cell stack designs include metallic interconnect plates, with grooved gas channels, made from high-temperature ferritic stainless steels[1]. During oxidation, these alloys form a beneficial conducting chromia-scale, but extended Cr-diffusion and oxide scale growth, limits the system lifetime[2]. Mn-Co-O spinel coatings significantly suppress the ionic diffusion and is industrially scalable using for example electrophoretic deposition (EPD)[3]. In this study, we investigate the effect of substrate groove curvature on the Mn-Co-O spinel EPD-coating after sintering. Inspection of the morphology reveals that cracks are formed in the coating (see stippled circle in Figure 1), deposited on Crofer 22 APU steel, at concave corners characterized by a small fillet radius (~15 µm). In contrast, coatings at concave corners with a larger radius (50-150 µm) and at convex corners (see inset Figure 1) are almost defect free. Finite element modelling of the mechanical stresses in the coating, demonstrates that concave corners are generally characterized by higher stress levels compared to convex corners (see Figure 2), due to thermal expansion coefficient mismatching. The inset in Figure 2 shows that the stress level scales inversely with the fillet radius. To prevent cracking in this ~20 µm thick spinel coating, we suggest that gas channel grooves are produced with a fillet radius larger than 50 µm.

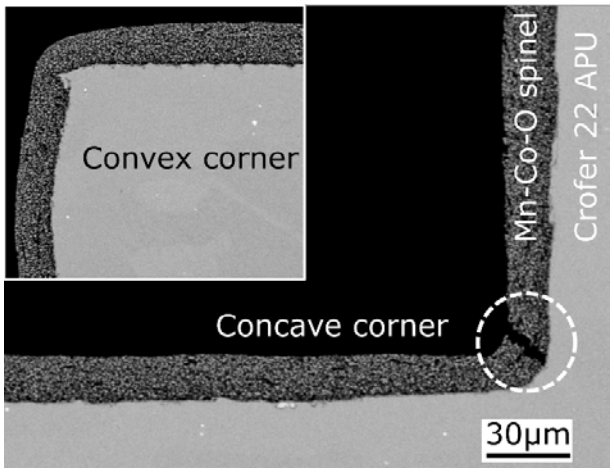

Figure 1: SEM image of the cross-section of the Mn-Co-O spinel layer on a grooved Crofer 22 APU substrate. Large image shows a concave corner with a typical small fillet radius. Inset shows a convex corner.

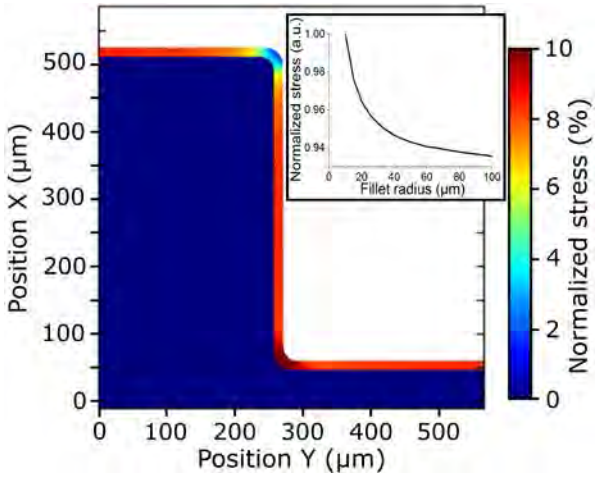

Figure 2: Finite element modelling (COMSOL Multiphysics) of the mechanical stress concentration for the coated steel substrate. Inset shows the mechanical stress as a function of fillet radius.

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Session

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Sandwich-like functionalized free-standing and flexible graphene papers for supercapacitors

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The development of flexible and free-standing electrodes is a key step for fabrication of flexible and compact electronic and energy devices which is of significant interests in portable electronics. This is increasingly demanded by modern electronics, portable medical products, and compact energy devices. Hybrid electrodes with functional nanocrystals anchored on carbon substrates are under intense research for a broad spectrum of applications in sensing, energy conversion and storage, and catalysis. Among carbon materials, graphene, consisting of a single-layer of sp^2-hybridized carbon atoms, has emerged as a new class of supporting scaffolds for nanocrystals because of a unique collection of structural and electronic properties such as large surface areas, chemical inertness, and superior electrical conductivity. As a two-dimensional (2D) transition metal dichalcogenide (TMDC), tin disulfide (SnS_2) is a promising material for multiple applications in supercapacitors, lithium ion batteries and photocatalysis due to its excellent optical and electrical properties. In this poster, we present a facile approach to the preparation of sandwich-like paper electrodes with Au nanoparticle-decorated reduced graphene oxide paper (r□OP-AuNPs) as substrates and 2D SnS_2 nanoflake-anchored reduced graphene oxide (SnS_2@r□O) nanosheets as high-performance supercapacitive material. The 2D self-assemblies of Au nanoparticles (AuNPs) on the surface of graphene papers can enhance electrode conductivity and facilitate electron transfer between r□OP and SnS_2@r□O, as well as serve as a strength reinforcing component by forming stable Au-S bonds. The proposed paper electrodes show the combined advantages contributed from both graphene paper substrates and self-assemblied AuNPs layers as well as could improve conductivity of 2D SnS_2 nanoflakes. Our results show the promise that this approach could evolve to be a universal strategy for practical fabrication of multifunctional flexible portable paper electrodes for energy storage and sensing devices.

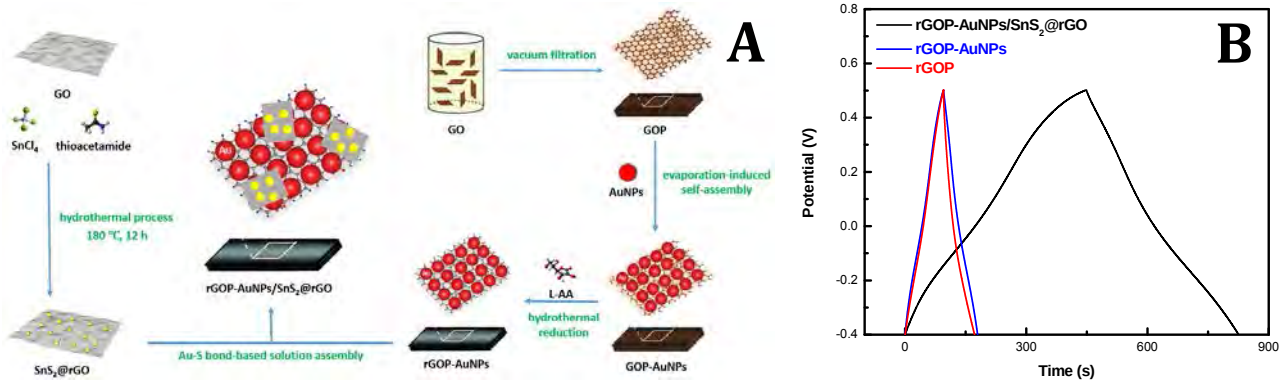

Fig.1 (A) Schematic for the fabrication process of rGOP-AuNPs/SnS_2□ rGO paper electrodes. (B) Charge-discharge curves of rGOP-AuNPs/SnS_2□ rGO, rGOP-AuNPs and rGOP at 0.5 A·g^{-1}.

Acknowledgments

This work was supported by DFF-FTP, the Danish Research Council for Technology and Product Science (to □.C., Project No. 12-127447). X.C. is grateful for the support from the Chinese Scholarship Council (PhD scholarship No. 201406170040).

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Detection of fungal growth and its influence on gypsum wallboard – in the process of creating sustainable building materials.

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Indoor fungi are a worldwide problem causing negative health effects for infected building's occupants and even deterioration of building structures. This research focuses on *Stachybotrys* and *Chaetomium* spp. growth on gypsum wallboard. It shows the influence of moisture and fungal mycelium influence on the gypsum wallboard microstructure via investigation of the material using micro-computed tomography (microCT) (Figure 1) and fungal mycelium penetration of the material (Lewińska et al., 2016a). From XRD and solid-state NMR results one can deduce that these fungi need amorphous cellulose and hemicellulose for their growth.

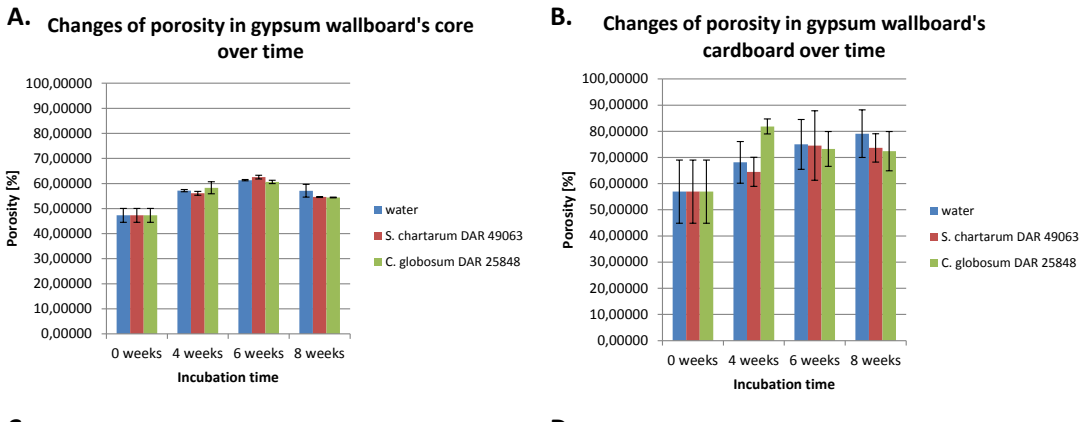

Figure 1. Water and fungal growth influence on porosity of core (A) and cardboard (B) from gypsum wallboard.

Furthermore, since different fungal species affect buildings and their inhabitants differently, rapid and accurate identification of fungi to the species level is essential for health risk assessment and building remediation. One of the fastest and most reliable methods is DNA barcoding. This study proposes two promising candidates for *Stachybotrys* and *Chaetomium* spp. - *hogA* and *h3-h4*, as well as the rapid novel protocol for direct identification of *Stachybotrys* and *Chaetomium* spp is introduced (Lewińska et al., 2016b).

This research not only uncovers new insight about the growth of filamentous fungi in damp building materials but also give the direction for the future research. It also brings us closer to the dream of fungi free and sustainable building materials.

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Imaging the Liquid Processes via *in-situ* Transmission Electron Microscopy

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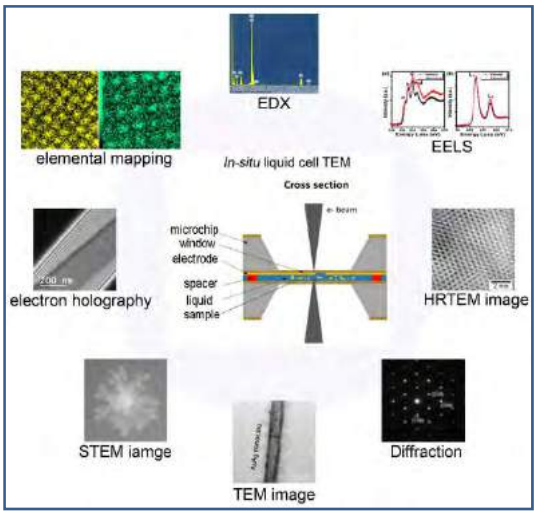
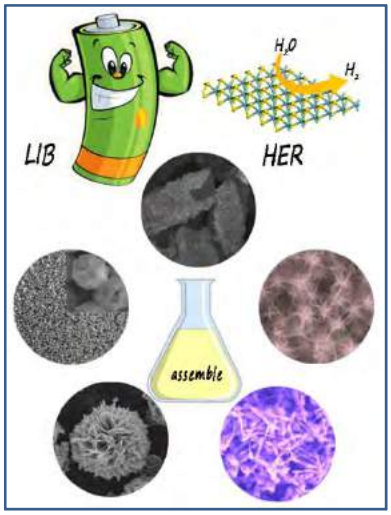
In-situ liquid cell transmission electron microscopy (LC-TEM) technique provides a unique ability to observe a wide range of liquid processes, such as crystalline nucleation and growth, electrochemical reactions, and bio-mineralization, within the fields of physics, chemistry and biochemistry.[1] The applicability is restricted by the fact that the electron beam has a so far not well quantified but strong influence on the sample [2] and the achievable image resolution is limited.[3] In this work we aim to overcome the limitations of the current LC-TEM method by fabricating unique microchip systems based on suspended nanochannels and microelectrode design to achieve atomic scale image resolution, and quantitative studying the complex electron beam effects in solutions *via* electrochemical measurements. It will provide new opportunities to study important liquid processes with emphasis on hydrothermal synthesis, electrodeposition, and water splitting by combining the spectral and imaging techniques of LC-TEM. Based on the gained fundamental knowledge and devices, we can study the electron holography in liquids,[4] which will likely provide a completely new liquid TEM imaging modality, and hopefully reveal both fundamental aspects of electrochemical systems. The present work should lead to LC-TEM being a core method to study nanoscale liquid processes.





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Electrodeposition of metallic 3D surface-profiles for superconductor tapes

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A recently introduced 3D surface-profile technique, i.e. the two level undercut-profile substrate (2LUPS) concept[1-3], for production of multi-filamentary high-temperature superconductors is investigated, applying electrodeposition to form 3D surface-profiles. Reducing the superconductor filament width effectively reduces alternating current hysteretic energy losses[4], and enables manufacturing of magnetic field-stable high temperature superconducting magnets[5]. The 2LUPS concept is based on two levels of plateaus

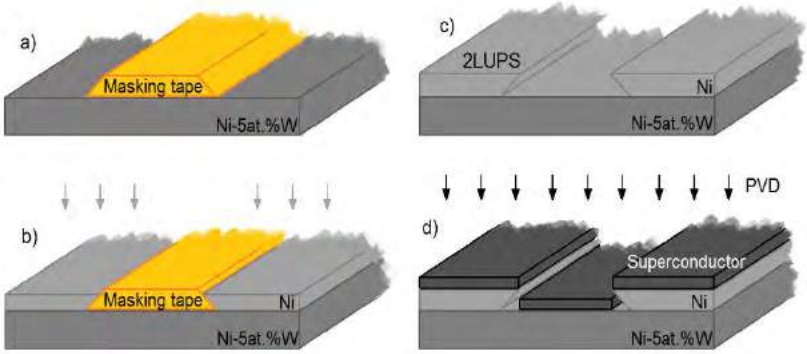

Figure 1: Schematic presentation of multi-filamentary coated conductor fabrication using electroplated two level undercut-profile substrates.

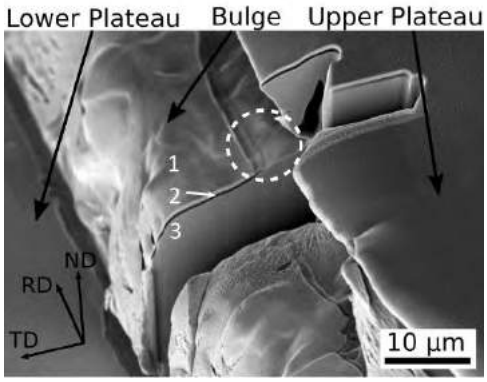

Figure 2: SEM image of an undercut-profile after focused ion beam milling. Center bulge is an effect of the tape glue. The image is tilted 36°.

connected by an undercut-profile, and is in this study fabricated using tape masking and Ni-based electroplating on a Ni-5at.%W substrate (see Figure 1a-c). The undercut-profiles enable self-formed and physically separated superconductor filaments during physical vapor deposition (PVD) as shown in Figure 1d. A Ni electroplate-based 2LUPS sample, prepared with a 400 nm thick SiO layer and a 400 nm thick Ag layer ("2" and "3" in Figure 2, respectively), is used to verify the shading effect of PVD deposited layers. Inspection of the 2LUPS cross-section using focused ion beam milling and scanning electron microscopy reveals an undercut-profile length of ~6-7 µm, and documents the physical separation (white stippled circle in Figure 2). The individual Ag filaments (representing the superconducting layer) are also observed to be electrically insulated with a resistance of ~26 Ω obtained across filaments, using four-point-probe I/V measurements, which corresponds to the electrically insulating SiO layer. Accordingly, we expect that these new electroplated 3D surface-profiles will also enable filamentization of superconductors produced by PVD.

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Effect of pectin and hemicellulose removal from hemp fibers on the mechanical properties of unidirectional hemp fiber/epoxy composites

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Hemp (*Cannabis sativa* L.) is one of the world's oldest cultivated and the most widely used industrial crops. Hemp bast fibers have high potential to substitute synthetic materials (e.g. glass fibers) in polymer matrix composites, but some pretreatments are required to increase the bonding between natural fibers and polymers to eventually improve the mechanical performance of natural fiber reinforced polymer composites. The objective of this study was to investigate the effect of pectin and hemicellulose removal from hemp bast fibers on the mechanical properties of unidirectional hemp fiber/epoxy composites. Pectin removal by EDTA and endo-polygalacturonase (EPG) removed epidermal and parenchyma cells from hemp fibers and improved fiber separation. Hemicellulose removal by NaOH further improved fiber surface cleanliness. Removal of epidermal and parenchyma cells combined with improved fiber separation decreased composite porosity. As a result, composite stiffness and strength increased (Fig. 1). Hemicellulose removal increased composite stiffness (Fig. 1), but decreased composite strength due to the disruption of interlocked network of cellulose and hemicellulose (Liu et al. 2016).

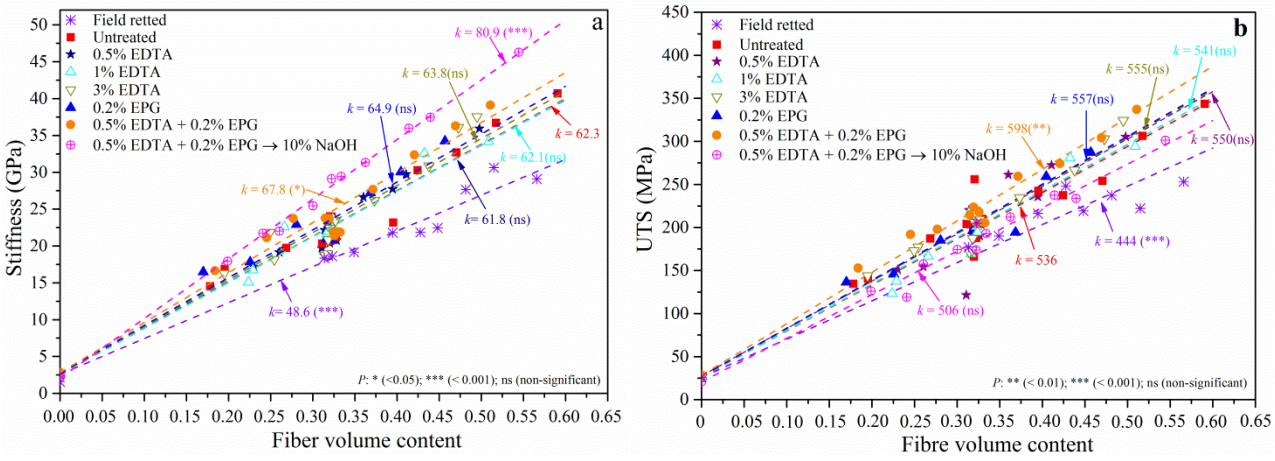

Fig.1. Stiffness (a) and ultimate tensile strength (b) of composites reinforced with differently treated fibers.

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Mechanical Characterization of Energy Materials at DTU Energy

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Due to the ever growing demand for sustainable energy alternatives, increasing the efficiency as well as reliability of energy conversion and storage technologies is becoming paramount challenge for the research community in the field. To achieve this, the innovation of new material systems should go hand in hand with understanding and improving their mechanical reliability at operational conditions. With this regard, DTU energy has a dedicated team and facilities working on characterization of metallic as well as ceramic materials used in energy conversion and storage technologies. The poster presents the unique capabilities in the department including high throughput and high temperature strength and deformational behavior characterization of materials in a controlled atmosphere. The characterization techniques mainly focus on materials being developed to be used in solid oxide fuel or electrolysis cells, oxygen or gas membranes, etc.

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Oxidation of lignin in hemp fibres by laccase: effects on mechanical properties of hemp fibres and unidirectional fibre/epoxy composites

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Hemp fibres (*Cannabis sativa*) are suitable as reinforcement in strong biocomposites because the cells in the bast fibres are aligned as long, robust structures that have a high strength to weight ratio due to the cellulose content. These fibres are mainly composed of cellulose, hemicellulose, lignin, and pectin. Laccase enzymes (EC 1.10.3.2) are capable of polymerizing aromatic substances such as lignin resulting in cross-linking. The polymerization aspects of laccase treatment were investigated in this study with the effect on stiffness of hemp fibre/epoxy composites in focus.

Laccase treatment on top of 0.5% EDTA + 0.2% endo-polygalacturonase (EPG) treatments increased the mechanical properties of hemp fibres and fibre/epoxy composites. Comparing all fibre treatments, composites with 0.5% EDTA + 0.2% EPG + 0.5% laccase treated fibres had the highest stiffness of 42 GPa at a fibre volume content of 50% (Fig. 1a). The thermal resistance of hemp fibres increased after laccase treatments, and the maximum degradation temperature increased about 5 °C (Fig. 1b). Cross-linking of hydroxycinnamates by laccase was not observed. Oxidation of lignin-OH groups by laccase was observed. We suggest that the increased mechanical properties of hemp fibres and fibre reinforced composites were due to laccase catalysed polymerization of lignin moieties in hemp fibres (Liu et al., unpublished).

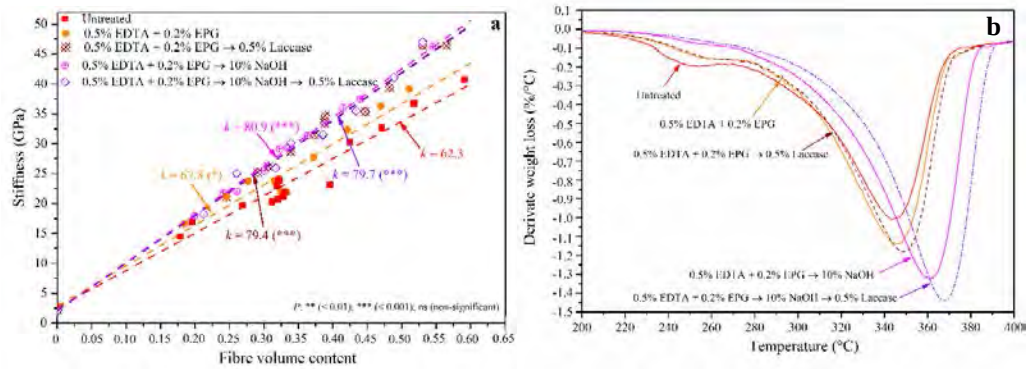

Fig.1. (a) Stiffness of composites reinforced with differently treated fibers and (b) Thermogravimetric analysis for derivatives of weight (%) vs. temperature (°C) of untreated and differently treated hemp fibres.

Reference: Liu, Baum, Odermatt, Berger, Yu, Zeuner, Thygesen, Holck, Meyer, 2016, Oxidation of lignin in hemp fibres by laccase: effects on mechanical properties of hemp fibres and unidirectional fibre/epoxy composites. Submitted to Composites Part A.

Bottom up design of a novel CuRu nanoparticulate catalyst for low temperature ammonia oxidation

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Ammonia has been considered as a renewable and carbon free energy source. Aside from hydrogen, ammonia is the only carbon-free energy vector for transport application. As 26% of all CO_2 is emitted from transport sector, without reducing the emission from the transport sector, it will be impossible to significantly reduce overall CO_2 emission. Ammonia is the second most produced chemicals in the world. It has the lowest cost per GJ of energy among all the conventional fuels[1]. It has been described as an important chemical storage of hydrogen that can transform the world to a low-carbon economy. Ammonia can also be produced with no carbon footprint at all using e.g. wind or solar energy. The decentralized small scale ammonia production units developed by Reese et al . and Proton Ventures can be a good way to store electrical energy in liquid chemical. Even though ammonia cracking in combination with low temperature fuel cells have long term potential in automotive applications, in short-term, the most attractive option is direct ammonia combustion. Ammonia is also combusted to generate hydrogen via ammonia cracking and auto thermal reforming. However the challenges of homogeneous ammonia combustion are high ignition temperature, low combustion rate and N_2O and fuel NOx production. So, there is a need to develop new ammonia combustion system. One possible way to avoid these issues is catalytic combustion which has many advantages over conventional non-catalytic combustion, as ignition temperature is decreased and NOx emission is reduced because of the low operating temperature[11] . The combustion reaction is also easier to sustain for catalytic reaction.

In this study we present a bottom up approach to design a novel core-shell nanoparticulate catalyst of ruthenium (Ru) and copper (Cu). The CuRu catalyst invented in this work has proven to be superior in terms of catalytic activity towards ammonia oxidation compared to both copper and ruthenium. A systematic surface scientific investigation of thin films and supported nanoparticles have elucidated the reasoning behind activity enhancement.

Catalyst for methanol synthesis prepared by deposition precipitation

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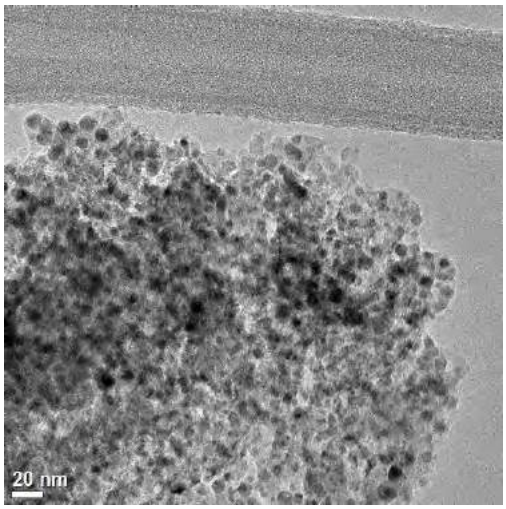
Methanol is a vital feedstock for the chemical industry with an annual production of approximately 70 million tons (2015 [1]). Conventionally a $Cu/ZnO/Al_2O_3$ catalyst operated at 50-100 bars at 200˚C-300˚C is used [2].

This study investigates, how Ni_5Ga_3 catalyst particles supported by silica (SiO_2) facilitate a low-pressure CO_2 hydrogenation process:

$$CO_2 + 3\,H_2 \leftrightharpoons H_20 + CH_3OH$$

Potentially this process allows intermittent renewable energy to be stored efficiently through first generation of hydrogen from e.g. water splitting and second by hydrogen conversion to methanol. Simultaneously the process mitigates the green-house effect caused by CO_2 and create a fossil-free pathway for generation of fuels and chemicals.

Theoretical studies [3] show, that the Ni_5Ga_3 catalyst exhibits promising properties in terms of methanol activity, stability and selectivity. Catalysts with three different metal loadings of 8.5 wt.%, 16.7 wt.% and 29 wt.% are prepared using the deposition precipitation (DP) method. Formation of the Ni_5Ga_3-phase is confirmed for all metal loadings by X-ray diffraction (XRD). Activity measurements are performed using a plug-flow-reactor (PFR), where the effluent gas is analyzed by gas chromatography (GC).



The methanol yield for the 16.7 wt.% and 29 wt.% are similar low (peak around 0.02 mol%), whereas the 8.5 wt.% is negligible small.
The low methanol production for the two highest metal loadings can partly be accounted for by too large particles observed by transmission electron microscopy (TEM) characterization. For the lowest metal loading the Ni_5Ga_3-phase purity is less pronounced.

Further work will optimize this firsthand DP catalyst synthesis. If successful the catalyst may solve some of the major obstacles, the world faces in the transition from a fossil-fuel based society to a green, fossil-free and sustainable society.

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Figure: TEM Micrograph for a catalyst with metal loading of 8.5 wt.%.

Recycled organic building materials are prone to fungal growth

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Fungal growth in buildings is an increasing problem worldwide and with dire consequences both in human and economic terms. Otherwise healthy people experience health problems (headaches, respiratory problems and mucosal irritations) when they live or work in fungal contaminated buildings. Asthmatics and allergy sufferers have their symptoms exacerbated, while hypersensitive people can experience rashes and nose bleeds even after a short stay. The consequences for society are extensive sick leave and the costly renovation of fungal contaminated estates and institutions. The renovation of a single-family house can easily cost several hundred thousand DKK, but a school can easily run up into double-digit millions. Fungal growth is not limited to any specific type of building, but can be found in old buildings and new constructions, in tower blocks and bungalows, in private homes and public institutions.

Organic building materials, such as gypsum wallboard, plywood, OSB, chip wood and paper wool, are popular, because they are cheap, lightweight and flexible. They are, however, also very susceptible to fungal growth, if the buildings are badly designed, shoddily build or used wrongly. Salvaged wood, cardboard and paper are often recycled and manufactured into new building materials, but research has shown that these materials often are ridden with fungal growth when they are collected or become so when stored prior to production (Andersen et al. 2016).

The demand for green and sustainable building materials is increasing and recycling is one of the few options, since both wood and gypsum are limited resources. However, the building materials of the future must not only be affordable and safe, but also robust and resistant to fungal growth.

At *Fungal Degradation* we work on controlling and preventing fungal growth in indoor environments. We employ the Hazard Analysis and Critical Control Points (HACCP) approach to find the entry points where fungal spores are introduced and study the conditions where fungi grow and proliferate. We also test methods and processes to reduce the risk of fungal contamination and eliminate production of mycotoxins.

Cardboard with growth of *Stachybotrys Chartarum* for recycling

Andersen B, Dosen I, Lewinska AM, Nielsen KF. (2016).Pre-contamination of new gypsum wallboard with potentially harmful fungal species. Indoor Air. DOI: 10.1111/ina.12298.

Session

P

Oral Presentations

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Adhesion layer investigation with complementary characterization methods for energy loss reduction in electronic nanodevices

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Metallic adhesion layers (Ti, Cr) have been introduced in different applications and research areas (e.g. semiconductors, plasmonics, metamaterials and 2D materials) to provide an enhancement of metal thin-film adhesion to dielectric or semiconductor substrates. Currently the thicknesses of adhesion layers and functional metal thin-films (over-layers) have reached comparable values (tens of nanometers), leading to a possible influence of the adhesion layer on the thin-film structure. Nanostructure of thin-films is an important microscopic property as it is directly connected to macroscopic physical properties, i.e. electrical conductivity. Comprehension of the adhesion layer dependence of thin-film nanostructure could have an important impact on fabrication of more sustainable nanodevices, having superior electrical performances and lower energy losses, reducing in this way energy consumption and impact on the environment.

In the present investigation Ti and Cr adhesion layers have been studied using micro 4-point probe (µ4PP) and transmission Kikuchi diffraction (TKD) to study their effect on electrical conductivity and nanostructure of Au ultra-thin films. Micro 4-point probe (µ4PP) is performed inside a dedicated SEM in order to visualize any thin-film damage during measurement, as standard 4-point probe (4PP) measurement would scratch the delicate thin-films. TKD is a material characterization technique used to visualize crystal structure, crystallographic orientation or domain/grain dimensions in materials with nanoscale order e.g. ultra-thin films and nanoparticles [1]. Fig. 1 shows nanostructure of the samples acquired with TKD. Comparison of 20nm Au sample (A) and 2nm Ti 20nm Au sample (B) shows a reduction of film grain size. We attribute this variation to the presence of the adhesion layer.

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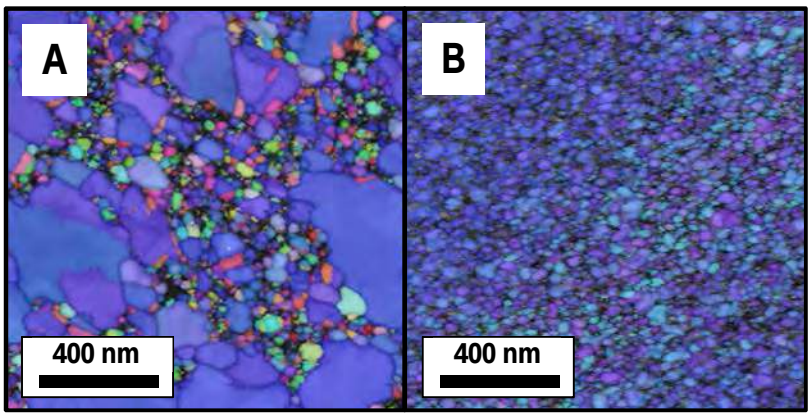

Figure 1 – TKD images of 20nm Au (A) and 2nm Ti 20nm Au (B) samples. Au sample shows high grain size dispersion. We observe a general decrease in grain size and dispersion for the sample with Ti adhesion layer.

Sustainable Electrochemical Hydrogen Production

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Molecular hydrogen (H_2) is one of the world's most important chemicals with a global production rate of approximately 50 billion kg per year. Today hydrogen is mainly used for petroleum refining and for synthesizing ammonia-based fertilizers but hydrogen also hold promise for the transportation sector using fuel cell vehicles. As hydrogen is mainly produced from fossil fuels, developing an alternative, renewable pathway to produce H_2 in a cost-competitive manner would have a significant impact in reducing fossil fuel consumption and CO_2 emissions. One attractive pathway for clean hydrogen production is through electrochemical processes coupled to renewable energy sources such as wind or solar.

The hydrogen evolution reaction (HER, $2H^+ + 2e^- \rightarrow H_2$) constitutes half of the water splitting reaction. To increase process efficiency, active catalysts for the HER are needed. Currently platinum is the best known HER catalyst as only small overpotentials are required to drive high reaction rates, but the scarcity and high cost of Pt may limit its widespread technological use. This has sparked a search for Earth-abundant catalysts that potentially could replace Pt - a search where the development of molybdenum sulfide (MoS_2)-based HER catalysts serves as an excellent example of theory-guided discovery and design of new electrocatalysts.

For decades, MoS_2 was believed to be inactive for the HER. However, inspired by hydrogen-producing enzymes such as hydrogenase and nitrogenase in nature, theoretical calculations predicted the edges of MoS_2 layers to be active. Guided by these calculations, several nanostructured MoS_2 catalysts have been synthesized to expose edge sites. In my talk, I will show this extraordinary development of non-precious metal HER catalysts and highlight a specific example of one such catalyst; $[Mo_3S_{13}]^{2-}$ nanoclusters.

Development of catalysts for electrochemical hydrogen production. *Left loop:* The interactive and interdisciplinary loop for discovering new catalysts in a rational manner. *Right loop:* Electrochemical conversion of water to hydrogen using energy from renewable sources.

Design for Biodegradability: the case of the Green Fiber Bottle

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Biodegradation is the degradation of materials by microorganisms. It is influenced by many factors, including exposure conditions (such as temperature and humidity) and material properties (such as chemical structure and superficial area). Despite its importance in a Circular Economy and sustainability context, there is currently a lack of knowledge in the literature on how to design biodegradable products, as previous work on biodegradation has not targeted product developers.

Design for Biodegradability guidelines are presented in this research, and consist of five steps: 1) Material Selection, 2) Coatings and Additives; 3) Biodegradation optimization; 4) Test preparation; and 5) Test and Certification (Figure 1).

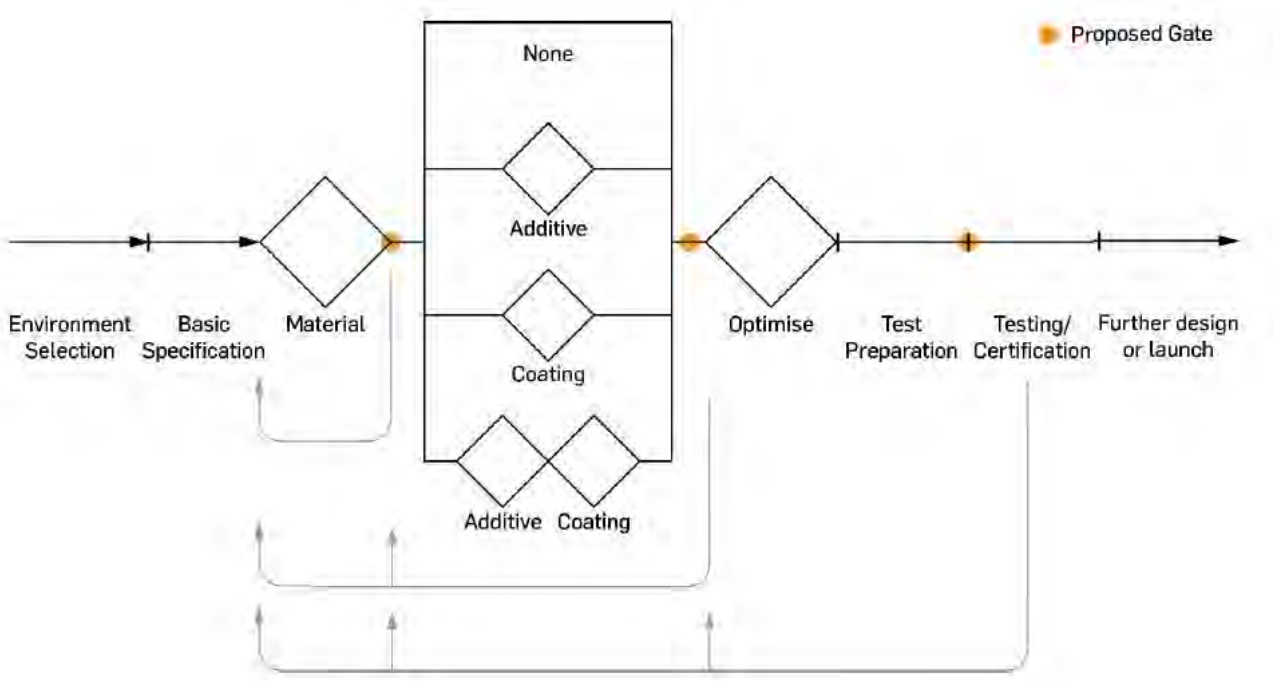

Figure 1: Guidelines for Design for Biodegradability

The evaluation of the usefulness of the proposed guidelines was performed by their application into the Green Fiber Bottle project, which is being developed by a collaboration between Carlsberg, ecoXpack and DTU for the development of a biodegradable beer bottle. Based on the application of the guidelines, the usefulness and applicability of the guidelines were demonstrated.

Discovering Challenges in Fabrication of Nanostructured c-Si Solar Cells with Metal Oxides Carrier Selective Contacts

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A photovoltaic cell provides direct conversion of solar in to electrical energy. Most modern solar cells are based on silicon due to well-developed technology, high efficiency, and high reliability and relatively low cost. In this research, our approach is based on nano-texturing of the crystalline silicon (black c-Si) with reactive ion etching (RIE)[1] and KOH techniques, ALD deposition of titanium oxide (TiO_2)[2] and RF magnetron sputtering of nickel oxide (NiO) films as carrier selective contacts[3,4]. Black c-Si technology allows reaching reflectivity below 1%. TiO_2 is a wide band gap semiconductor, transparent to photons with energy below 3.2 eV, it is a n-type electron selective layer. NiO is also wide bandgap (3.4 eV) p-type semiconductor, complementary to TiO_2, allowing only hole transport. Further fabrication process included RCA cleaning of nanostructured surfaces and deposition of Al_2O_3 passivating film with atomic layer deposition (ALD)[5]. In order to create local area carrier selective contacts, standard photolithography was used to make opening in Al_2O_3 film. 5 nm of TiO_2 film was deposited with ALD at 80°C. The second photolithography was applied form back contacts openings priory RF sputtering of Ni in O_2 and Ar plasma and NiO film deposition. Front contact grid was formed with the third photolithography and liftoff process. Both, front and back contacts were deposited with electron beam method with a thickness of 600 nm of Al.

In summary, characterization results of the fabricated cell helped to define a number of challenges:

- High surface damage during RIE process and therefore high recombination losses
- ALD Al_2O_3 process shows low passivation quality due possible low quality of TMA precursor.
- ALD TiO_2 films were deposited with $TiCl_4$ precursor, which is also lacking good passivation quality, TiO_2-Si form leaky diode due to interface defects and some Ti metal traces at the interface.
- NiO RF sputtering damages Si due to the nature of sputtering process. The stoichiometry of NiO film sputtered from Ni in O_2 and Ar plasma is not predictable and can be modified with a small parameters shift.
- Al electron beam deposition possibly damaging TiO_2 5nm film, which leads to diode leakage

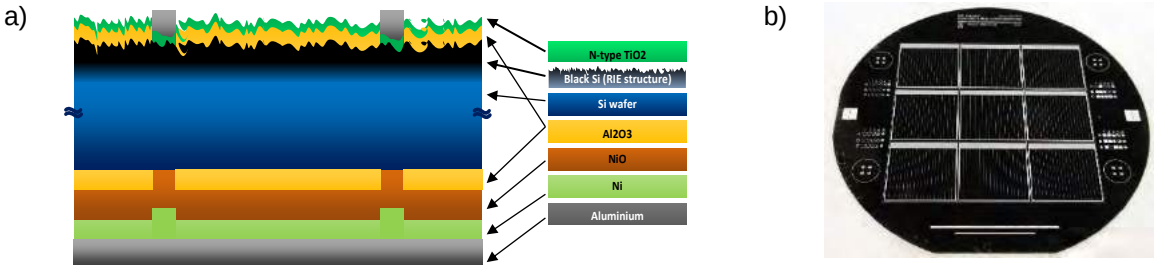

Figure 1. Nanostructured c-Si solar cells with metal oxide carrier selective contacts: a) cross-section schematics of the solar cell architecture, b) photo image of fabricated black silicon solar cells with carrier selective contacts

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Session

P

Laptop Presentations

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Material Removal Mechanisms Analysis in the dry Electrical Discharge Machining and Possibilities for Micro-machining Applications

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In dry electrical discharge machining (EDM), mineral oil-based liquid dielectric is replaced by gaseous dielectrics such as oxygen and inert gases. In order to use the eco-friendly dry EDM technology for micro-machining applications, particularly involving generation of complex 3D features with high accuracy, an understanding of the mechanisms of material removal is essential. The results of a single spark investigation in dry EDM at different energy levels (4.5 mJ and 324 mJ) and by employing external magnetic field of 0.1 T for improving the material removal in the process, are analyzed at a fundamental level. In this research, the crater radii and the rates of material removal in dry EDM and liquid dielectric EDM processes were related and compared considering the possibilities for scaling down to the micro-meter scale and beyond. At low input energies between 2 mJ and 14 mJ, the crater radius as well as the removal of material from the crater in dry EDM is higher, whereas at higher input energies between 28 mJ and 162 mJ, the liquid dielectric EDM yields a larger crater radius and a higher material removal. In single spark dry EDM, the crater diameter reduces by 40% and its depth appears to increase with the application of magnetic field around the single spark. The presence of a magnetic field helps removal of uniform material from a crater surface, during sparking in the liquid dielectric EDM conditions.

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Session

P

Poster Presentations

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Superhydrophobic Properties of Nanotextured Polypropylene Foils Fabricated by Roll-to-Roll Extrusion Coating

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Technologies for fabrication of biomimetic surfaces with superhydrophobic properties have gained considerable attention, due to the broad range of applications such as solar cells, self-cleaning fabrics, antireflective, antifogging and anti-ice materials. Fabrication of superhydrophobic materials usually requires initial structuring with a hierarchical micro- and nanopattern to increase surface roughness and a subsequent coating with low surface energy chemistry. The surface coating does however represent at least one extra fabrication step and is best suited for coating of solid surfaces, such as that of Si with perfluorodecyltrichlorosilane (FDTS). Enabling direct large-area surface texturing of intrinsically hydrophobic thermoplastics would be more feasible and lower the barrier for use of superhydrophobic materials for, e.g., self - cleaning applications.

Among technologies for large-area nanotexturing, roll-to-roll (R2R) UV-assisted nanoimprint lithography is the most established. A R2R method for production of large-area superhydrophobic surfaces should preferably have much higher productivity and allow structuring of common inexpensive and intrinsically hydrophobic polymers to gain practical relevance. An ideal material is isotactic PP, which has good hydrophobic properties, has low surface energy, and is inexpensive. In this research we report on R2R extrusion coating (R2R-EC)[1], as sketched in Figure 1a, for the manufacture of superhydrophobic surfaces in PP. R2R-EC is well established and widely used in the packaging industry for largescale fabrication of smooth polymer films.

We demonstrate the use of roll-to-roll extrusion coating (R2R-EC) for fabrication of nanopatterned polypropylene (PP) foils with strong anti - wetting properties[2]. The anti - wetting nanopattern is originated from textured surfaces fabricated on silicon wafers by a single-step method of reactive ion etching with different processing gas flow rates (70-50, 70-70, 70-90). We provide a systematic study of the wetting properties for the fabricated surfaces and show that a controlled texture stretching effect in the R2R-EC process is instrumental to yield the superhydrophobic surfaces with water contact angles approaching 160° and droplet roll-off angles below 10°.

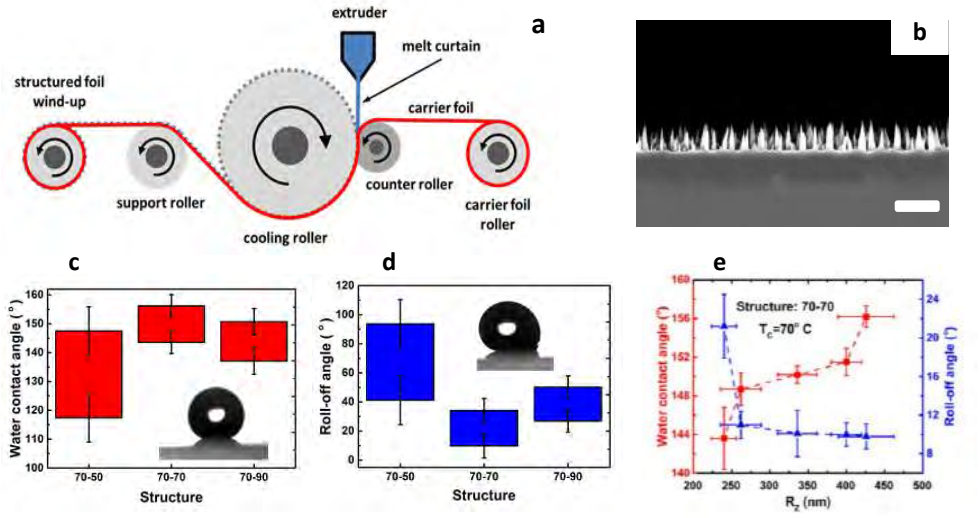

Fig.1 a) R2REC set up, b) SEM master cross section image, c), d), e) wetting properties of replicated PP foils

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Electrochemical Oxidation of Hydrocarbons for Green Chemistry

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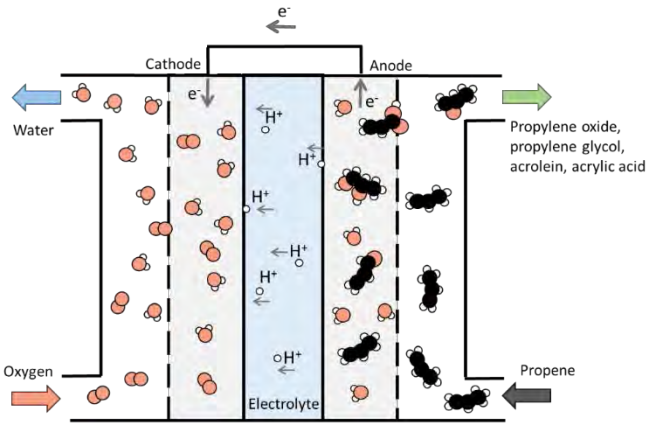
Abstract

The synthesis of many bulk chemicals as base materials for the chemical industry still relies on processes that were developed at the beginning of the last century. They often involve harmful chemicals or high temperatures and pressures which are not in agreement with green chemistry. One way to combat this problem is developing electrochemical processes suitable to replace the old techniques in a more sustainable way. In addition to avoiding dangerous chemicals and process conditions, the employment of electrochemistry also allows better tuning of the reaction conditions to increase selectivity. The focus of this project is on the electrochemical oxidation of propene. There are several oxidation products relevant for the chemical industry that are currently also produced from propene: Propylene oxide, propylene glycol, acrolein and acrylic acid. Propylene oxide is currently produced either by the chlorohydrin process, or by oxidation with organic peroxides. Acrolein is produced by gas phase oxidation of propene with oxygen at high temperature and pressure. Propylene glycol and acrylic acid are then produced from propylene oxide and acrolein, respectively.



Electrochemical oxidation of propene in a fuel-cell-type setup

It has been shown that in an electrochemical process in alkaline, aqueous electrolyte, high selectivity for propylene oxide can be reached.[1], [2] In acidic environment, on the other hand, selectivity is higher towards acrolein.[3]–[5] Optimization of the process parameters and development of new catalyst materials will lead to a better understanding of the reaction mechanism and clear the way towards a more sustainable process for generating propene oxidation products.

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Ice lithography: water-based nanopatterning

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Almost any micro- and nanostructure, such as the entirety of modern electronics, requires one and generally several lithography iterations where the desired features are defined in a sacrificial layer (resist) used in further processing. This is typically done using UV light but to overcome diffraction limits collimated electron beams are used to resolve nanometric resolution. A typical lithography process requires multiple different tools, engineered materials and abundant solvents to create, develop, and then remove the thin resist film on the desired substrate.

Ice lithography is a novel technique which doesn't suffer from these limitations. The role of resist is taken by water, deposited directly inside the electron beam chamber on a cooled substrate to create a thin ice film to be patterned [1]. No harmful chemicals or other tools are needed. Extremely high resolution was demonstrated, even on non-planar or fragile substrates which are a challenge for conventional techniques [2]. An in-situ metallization process allowed using the patterned ice to create seed layers for further processing or actual devices [3].

Here at DTU, we recreated an ice lithography setup to further explore this promising technology. A scanning electron microscope was modified for cryogenic operations and ice deposition (Fig.1) and can now be used to research applications in advanced nanofabrication and potential for high volume manufacturing.

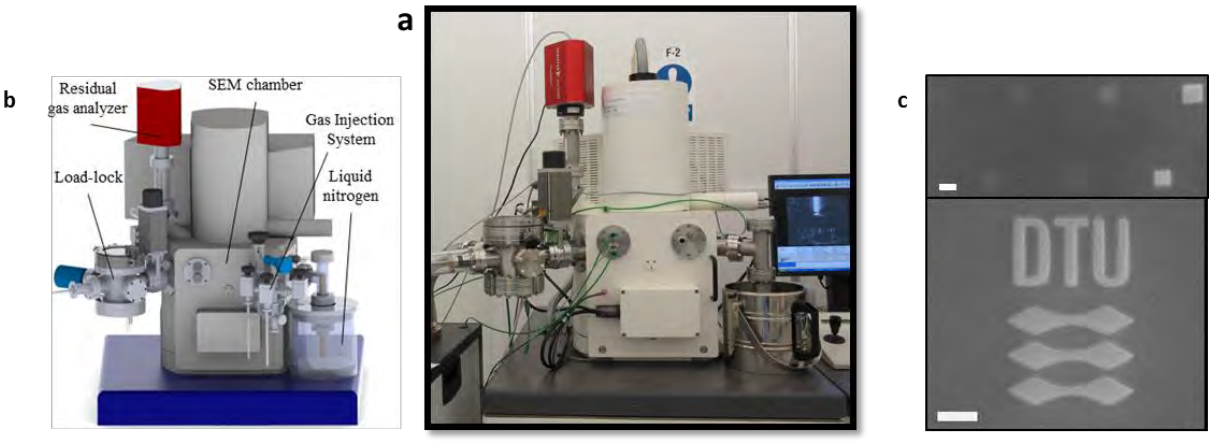

Figure 1 – Ice lithography at DTU Danchip. The modified SEM for ice lithography (a) and the original 3D model (b) used to design the custom parts produced in DTU Nutech's workshop. By progressively increasing the electrons delivered per unit area (c, top), the optimal dose is identified and used to reproduce arbitrary patterns on 100 nm ice films (c, bottom). Scale bars in (c) are 1 µm.

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Induction-Heated Hydrogen Production

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Hydrogen is widely used in the industry, mainly for production of ammonia fertilizer and hydrocracking in the petrochemical industry [1]. Minor applications include the food industry, hydrogenation reactions, metal processing and the growing market for fuel cells. The steam reforming reaction converts hydrocarbons (C_nH_m) and water to hydrogen, carbon monoxide and carbon dioxide, and is the main source of hydrogen production today [2]. The reaction is strongly endothermic and only efficient at large scale where the excess heat can be integrated into other processes.

Induction heating can supply the heat directly at the catalyst, improving efficiency and enabling a more compact reactor design, suited to small scale and on-demand production of hydrogen. With methane readily available by an already established infrastructure, an efficient catalytic system based on induction heating could provide on-demand hydrogen remote consumers, or be integrated in the energy network to store excess renewable energy as chemical.

The first step of the project is development of a CFD model (Computational Fluid Dynamics), to predict temperature profiles, efficiency and to some extend degradation mechanisms. This will later be held against experimental results from a bench scale reactor (currently under construction).

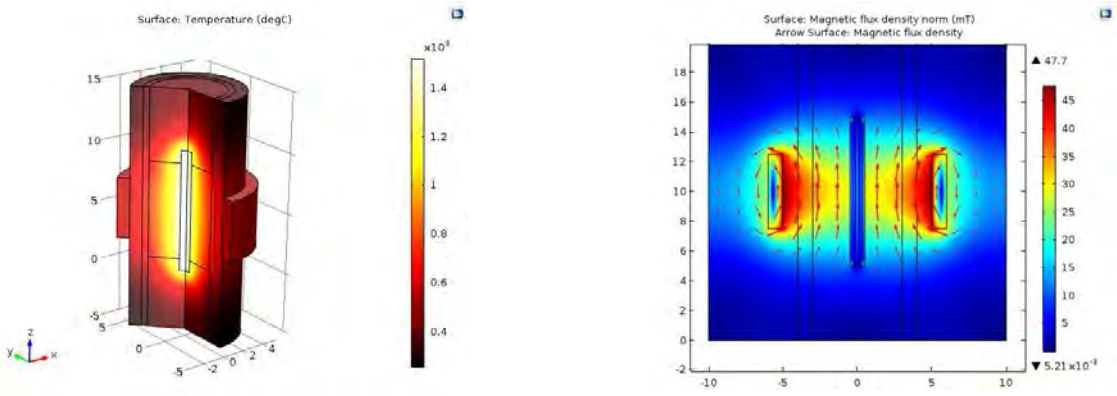

Figure 1: Examples of initial CFD simulations in COMSOL, displaying the temperature (right) and magnetic flux (left).

Once the system is operational and adequately efficient (>70%), optimization of system stability will be the main focus. Several degradation mechanisms from conventional steam reforming are well documented [2], such as carbon deposition and metal dusting, but no studies investigate the degradation related to repeated start and stop of the reactor, which may be very relevant for this particular system.

The goal of the project is establishing an understanding of the mechanisms in induction heated steam reforming, including heating mechanisms and degradation phenomena. The aim is to improve the catalytic material and the reactor design, in terms of conversion, stability, and energy efficiency.

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Acetate production enhancement from carbon dioxide reduction by using modified cathode materials in microbial electrosynthesis

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Microbial electrosynthesis (MES) is one of the emerging biosustainable technologies for the biological conversion of carbon dioxide to the value-added chemical precursor. The electro autotrophic bacteria fix CO_2 via Wood-Ljungdahl pathway, accepting the electron derived from the cathode in the bioelectrochemical System (BES). The MES reactor can power with the solar photovoltaic system and harvest light energy to multi-carbon compounds to make it artificial photosynthesis system. Nevertheless, chemical production rate should be optimized for the commercialization of MES technology. Interestingly, it has been demonstrated that the productivity was enhanced with the modified cathode surfaces by improving microbe-electrode electron transfer. Here, we have tested the different cathode materials for the improvement of acetate production from carbon dioxide and their behavior for the biofilm formation. Interesting, graphene based electrode materials has better performance on the acetate production and microbe-electrode interaction. Modification with three-dimensional metal-graphene networks increased the electrosynthesis rate of acetate from CO_2 by 10.2 fold compared with three-dimensional graphene network by using *sporomusa ovata*.

Keywords: - Microbial electrosythesis, CO_2 reduction, Acetate, Three-dimensional electrode, Graphene, *Sporomusa ovata*

Energy Saving on Cleanroom Fume Hoods

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As a rule of thumb, a standard fume hood consumes more electric energy per year as a private home [1]. This large amount of energy is mainly consumed by the ventilation system, which constantly has to pump air from the operator space in front of the fume hood through this and into the exhaust in order to prevent dangerous fumes from reaching the person working in front of the fume hood.

A fume hood in a cleanroom for micro- and nanofabrication is even more energy consuming, since the air being pumped through it has already been conditioned to be ultra-clean and have a very well-defined temperature and humidity. Proper conditioning of cleanroom air is very costly and it is therefore very important that as much air as possible be "saved" so it can be recycled. Since the air inside a cleanroom is changed over 200 times per hour, considerable savings are possible.

When the movable front window of a fume hood (often referred to as the "sash") is open, the air volume passing through it is considerably larger than when the sash is closed. It is thus important that the sash is only opened when an operator is working in front of the fume hood. All cleanroom users at DTU Danchip are taught that they should remember to close the sash after finishing their work. However, too many users tend to forget this basic rule, and that leads to excessive energy consumption.

Due to the above mentioned reasons, it was very important for DTU Danchip when ordering 18 new fume hoods and ventilated wet benches, that these be equipped with an energy saving mechanism. The energy saving mechanism consists of a passive infrared (PIR) sensor, a sash drive motor and an air flow regulator. If the PIR sensor does not sense any motion in front of the fume hood for more than 90 seconds, the motor will automatically close the sash and the air flow regulator will reduce the volume of air passing through the fume hood. Figure 1 shows a row of installed fume hoods – all of which are equipped with energy saving.

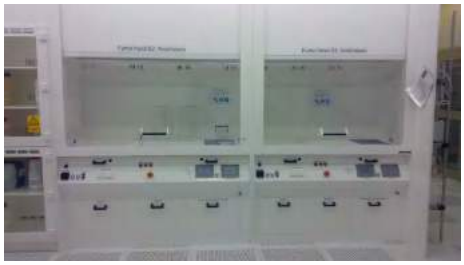

Figure 1: A row of newly installed fume hoods at DTU Danchip. All are equipped with energy saving.

[1] *Fume Hood Energy Usage and Incentivization,* Silas Hilliard

Framework for measuring the sustainability performance of ecodesign implementation

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Companies and academic studies are consistently reporting several potential business benefits gained from ecodesign implementation, such as increased innovation potential, development of new markets and business models, reduction in environmental liability, risks and costs, improvement of organizational brand and legal compliance, among others. However, there is a number of challenges that still hamper corporate adoption of ecodesign, mainly regarding the capture and measurement of the estimated business benefits. Furthermore, ecodesign efforts have been primarily evaluated in terms of environmental performance and product-related (technical) measures, such as shape, material and energy consumption. Because the ecodesign business benefits go beyond the pure environmental performance and its implementation should follow a consistent process-oriented integration, an approach based on the triple bottom line and focused on the managerial perspective is required to deriving a consistent business case for ecodesign.

This research aims at proposing a simulation-based framework geared towards laying out the fundamental rationale of the business case for ecodesign implementation. The study particularly builds upon the Ecodesign Maturity Model (EcoM2), a management framework that offers a systematic, step-by-step approach for the integration of ecodesign into product development processes. With more than 600 ecodesign practices systematized and organized according to maturity levels, the EcoM2 offers an application method with 4 steps, organized in two phases (**Figure 1**). The simulation framework draws upon the **current** and **desired capabilities** of ecodesign practices, and offers an integrative outlook into how capability building will potentially affect corporate indicators over time, such as revenue, market share, expenses, risk, employee productivity, among others. It is expected that decision makers use the business case simulator to assess the potential benefits of ecodesign and test multiple scenarios (what-if questions) with a view to deriving more robust implementation policies, in alignment with corporate sustainability strategy and main drivers.

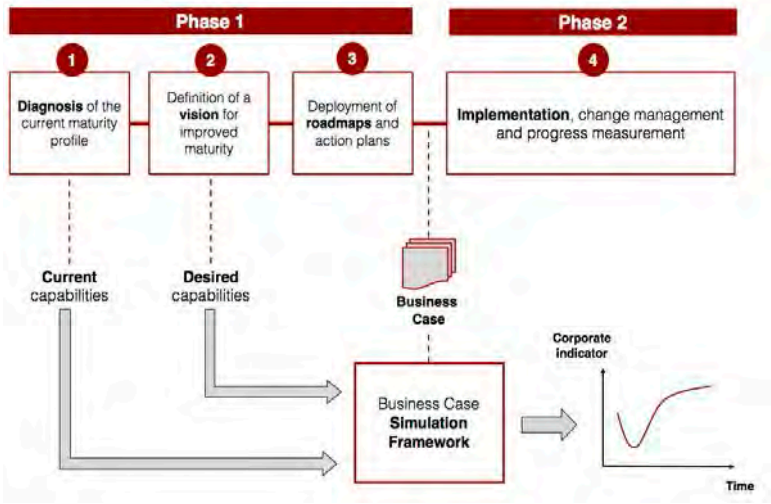

Figure 1 – Schematic representation of the use of the business case simulation framework within ecodesign implementation efforts

How to mature the abilities of companies to a successful transition to Circular Economy?

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Circular Economy is increasingly recognized as a promising approach to maximize value by increasing resource productivity, minimizing resource consumption and decreasing waste. The transition of manufacturing companies from a linear to a circular economy requires a systemic change in several organizational processes and functions: from strategy and business models to take-back and end-of-life management. To support the transition of manufacturing companies towards Circular Economy, we have developed a maturity-based approach that aids the development and implementation of strategic roadmaps and action plans towards circular economy. In this abstract, we present our analysis that resulted in the identification of twelve key management practices to manage the transition towards Circular Economy (Figure 1).

Industrial applications of the proposed maturity approach through a case study for theory testing indicate that it can effectively support companies to mature their abilities to embrace the Circular Economy.

A similar maturity-approach based on diagnosis, vision and roadmap development based on a gap analysis can be employed to any other strategic drivers linked to sustainable innovation that a given company might have.

Figure 1: Schematic representation of the maturity profile, showing the visualization of the gap between the as-is and to-be maturity profiles

Session

R

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An innovative process for biogas upgrading by the microbial electrolysis cell

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Biogas as an alternative energy source is getting more attention which can facilitate to reduce fossil fuel utilization and greenhouse gas emissions. However, biogas is a mixture of gases and typically composed of 60-70% v/v methane (CH_4) and 30-40% v/v carbon dioxide (CO_2), small amounts of hydrogen sulfide (H_2S) and other gases. Rude biogas exhibits a significantly low Wobbe index, heating value and energy efficiency which hinder its application. Therefore, CH_4 enrichment prior to use is crucial to improve the quality of biogas. In this work, a novel bipolar membrane-microbial electrolysis cell (BPMEC) was proposed to realize biogas upgrading. The system was composed of the anode, middle and cathode chamber which were separated by a bipolar membrane (BM) and an anion exchange membrane (AEM), respectively. With an external potential, water dissociation occurred and acid was produced in the middle chamber while electrolysis happened and alkali was generated in the cathode chamber. When rude biogas was injected into the cathode chamber, CO_2 was absorbed chemically into the solution and migrated via AEM as the form of CO_3^{2-} and HCO_3^- into the middle chamber where they reacted with H^+ and CO_2 was regenerated and released from the solution. The gas flow rates were varied, as well as the external voltage. Results revealed the highest cathodic pH was 10.03±0.21 and the lowest pH in the middle chamber was 1.34±0.21. The highest CO_2 removal efficiency can be reached at 98.76±1.32% and the maximum CH_4 content can be 98.13±1.12% with 19.64 ml/h gas flow rate and 1.2 V external potential. Organic matter was removed remarkably and COD of the last day was below 60 mg/l. Hydrogen (H_2) was produced and collected in the enriched gas which is another benefit of the system. This study provides a simple, efficient and sustainable way to extend the application of electrochemical technology.

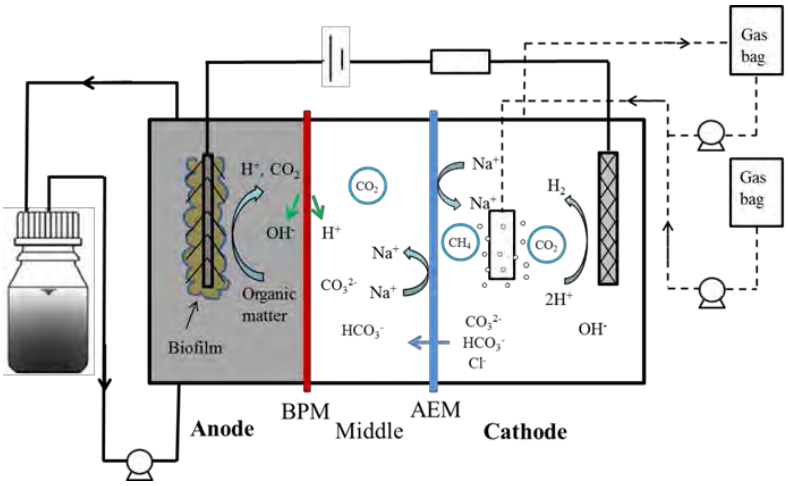

Fig. 1. The schematic diagram of the BPMEC system

Assessing environmental performance of hydrothermal carbonization of wet biomass at industry-relevant scales

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Hydrothermal carbonization (HTC) of wet lignocellulosic biomass is attracting attention as a biorefinery concept as it allows producing the carbonaceous material hydrochar and various organic chemicals (1). Hydrochar can be used as solid fuel for domestic heating. Here, we assessed hydrothermal carbonization (HTC) of green waste, food waste, organic fraction of municipal solid waste (MSW), and digestate using life cycle assessment (LCA) as a potential technology to treat biowaste (2). Key parameters for the modelling were based on measurements performed at a pilot plant at Ingelia S.L. (Valencia, Spain). The parameters for the full commercial-scale process were estimated from the pilot plant values using scaling factors that consider optimization and increased material needs for a full commercial-scale plant.

The results show that hydrochar produced from green waste performs best and second best in 12 out of 15 impact categories, including climate change, mainly due to low transportation needs of the biowaste and optimized pumping efficiency for the feedstock. By contrast, hydrochar produced from the organic fraction of MSW has relatively high potential impacts on human health and ecosystems caused by emissions of toxic elements through ash disposal. The greatest potential for environmental optimization for the HTC technology is in the use of heat and electricity with increasing plant size, but its overall environmental performance is determined in a given geographic location mainly by the energy sources that the hydrochar substitutes. When hydrochar replaces fossil coal as heat source, impact scores are within the range of existing alternative treatment options, suggesting that despite being a relatively immature technology HTC may be an attractive biorefinery concept for wet biomass.

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(2) Owsianiak, M., Ryberg, M.W., Renz, M., Hitzl, M., Hauschild, M.Z., 2016. Environmental performance of hydrothermal carbonization of four wet biomass waste streams at industry-relevant scales. ACS Sustain. Chem. Eng. doi:10.1021/acssuschemeng.6b01732

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R

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Novel bio-electro-Fenton technology for azo dye wastewater treatment using microbial reverse-electrodialysis cell

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Development of sustanaible technologies for treatment of recalcitrant pollutants such as azo dye containing wastewaters has long been of great interest [1]. In this study, we proposed an innovative concept of using microbial reverse-electrodialysis cell (MRC) based Fenton process to treat azo dye wastewater. In the MRC-Fenton process, the production of H_2O_2 which is the key reactant of fenton-reaction was driven by the electrons harvested from the exoelectrogens and salinity-gradient energy between high and low concentration salt water in MRC. Complete decolorization and mineralization of 400 mg L^{-1} Orange G (a synthetic azo dye) was achieved with apparent first order rate constants of 1.15 ± 0.06 and 0.26 ± 0.03 h^{-1}, respectively. Moreover, process parameters such as the initial concentration of orange G, initial azo dye wastewater pH, high concentration (HC) and low concentration (LC) salt water flow rate and air flow rate were all found to significantly affect the dye degradation. The MRC-Fenton system has several advantages compared to the traditional Electro-Fenton system, such as lower operational costs, higher efficiency, and higher safety level. Thus the MRC-Fenton system can provide an efficient and cost-effective system for the degradation of non-biodegradable pollutants.

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Statistical optimization of operating parameters for CSTR bioprocesses: the case study of glycerol conversion

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Statistical optimization is often applied for the improvement of biotechnological processes [1]. It is typically performed in batch mode, allowing for statistical independent experiments [2], higher amounts of replicates and faster operation times. However, optimal conditions obtained in batch conditions are not necessarily corresponding to the best ones in continuous mode. Moreover, the Hydraulic Retention Time, HRT, is another important factor that can be taken into account in continuous experimentation. For this reason a different approach was tested, namely performing statistical optimization directly in a continuous process.

The bioconversion of crude glycerol into 1,3 propanediol (PDO) and butyric acid by mixed microbial consortia was investigated as a case study. Each experimental run was performed for a period of 20 HRTs, in order to confirm the establishment of steady state and to demonstrate the ability of the system to maintain it. The average values of the model responses obtained during the steady state (corresponding to approximately an operation period of 6 HRT) were used for the statistical model. An Inscribed Central Composite (ICC) Design was used to optimize 3 key factors (pH, glycerol concentration in the feed and HRT) and maximize productivity of PDO and butyric acid, with the help of the software Unscrambler X 10.3.

The results showed a model with a complex interaction between the key factors, which implied a very careful choice of operating parameters. In fact, lower pH required low glycerol concentration (10-20 g/L), while higher pH showed better productivities with high substrate concentration (40-50 g/L). The model further showed the need for a fine tuning of HRT in combination with the other parameters, in order to maximize productivities and avoid cells wash out. This confirmed the importance of CSTR optimization. On the other hand, the optimization of HRT presents a further challenge, since it is not possible to obtain a classical peak, but only a maximum value, before cell wash-out. To avoid this problem, preliminary tests and kinetic characterization of the consortium turned out to be fundamental to choose the proper experimental range. Maximum experimental glycerol consumption rate reached 137 g/L/d, followed by a production rate of 59 g/L/d, 15 g/L/d and 11 g/L/d, for PDO, butyric acid and acetic acid, respectively. This corresponded to a 5-fold increase compared to steady state results in standard fermentation conditions prior to optimization (12h HRT, 10 g/L glycerol, pH 5.5). Maximum predicted productivities reached 77 g/L/d for PDO (pH 6.43, HRT = 7.85, Glycerol = 41.36) and 21 g/L/d for butyric acid (pH 6.54, HRT = 7.84, Glycerol = 46.84). Future steps include model validation under the abovementioned conditions.

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SYNFERON – An Alternative Approach to the Production of Biofuels

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The ever increasing demand of energy along with the rise of greenhouse gas emissions and waste production on a global scale make evident the need for a transition to a more sustainable bio-based economy. In this sense, mixed culture biotechnology presents a high potential for contributing to this transition as it accomplishes a dual function of waste treatment and production of renewable energy. This emerging field of study is currently expanding beyond the conventional anaerobic digestion process towards the development of new technological platforms for the production of a variety of chemicals and fuels [1-2]. Syngas fermentation is an example of such innovative platforms that has recently emerged as an alternative to catalytic syngas conversion processes. The production of biofuels through fermentation of syngas has significant advantages over the conventional chemical catalytic processes including higher specificity in the conversion, better tolerance to gas impurities and flexibility in the H_2/CO ratio avoiding costly syngas reforming processes. However, the challenges of the existing syngas fermentation technologies such as the necessity to maintain sterile conditions and the limited mass transfer of sparingly soluble syngas compounds (CO, H_2) to the water-based microbial cultures need to be addressed in order for this technology to be applicable.

SYNFERON aims at integrating the mixed culture approach and the syngas platform along with the design of a novel reactor. The implementation of a mixed culture approach provides a series of potential advantages such as non-sterile operation and the adaptability of microbial communities to sudden changes of the operational conditions, leading to a more stable bioreactor performance. Research in this part will focus on the design of microbial enrichment strategies, the kinetic characterization of the microbial groups composing the consortia, and the selection of key operating parameters for optimal performance of the enriched microbial consortia. On the other hand, the selection of an appropriate bioreactor configuration based on a packed bed reactor design will contribute to overcome the mass transfer limitations and achieve high cell density for efficient syngas fermentation.

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Enzymatic Modifications Based on the Surroundings of Cofactor

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Redox-active enzymes are widely present in the eukaryotes assisting the electron transfer process involving respiration and photosynthesis. The difference of the onset potentials of the enzymes is the pumping power of the electron transfer crossing the membranes. In social production and life, enzymes play important role in immunoassay, and energy transformations.[1] For example, horseradish peroxidase is applied to detect H_2O_2, metal ions, protein and DNA through the biomarkers. Glucose dehydrogenase or alcohol oxidases are applied to construct the biofuel cells to create the electrical energy by the consumptions of the cheap and clean fuels. The modifications to the enzymatic properties are important topics to improve the selectivity and activity of the enzymes, and increasing the loading amount of enzymes on the cathodes.[2] It includes the mutations of the key residues surrounding the cofactor, and altering the structures of cofactors. Herein, we will study the electrochemical properties of DNAzyme which is constructed with guanine-rich DNA single strand and hemin. As shown in **Figure 1**, the DNA strand folds into G-quartet structure in the presence of K^+ and further interacts hemin molecule by the *л-л* stacking force.[3] The G-quadruplex-hemin complex possess the enzymatic activity as cytochrome c, which is expected applied in bioanalysis and biofuel cells due to its stability and smaller size.

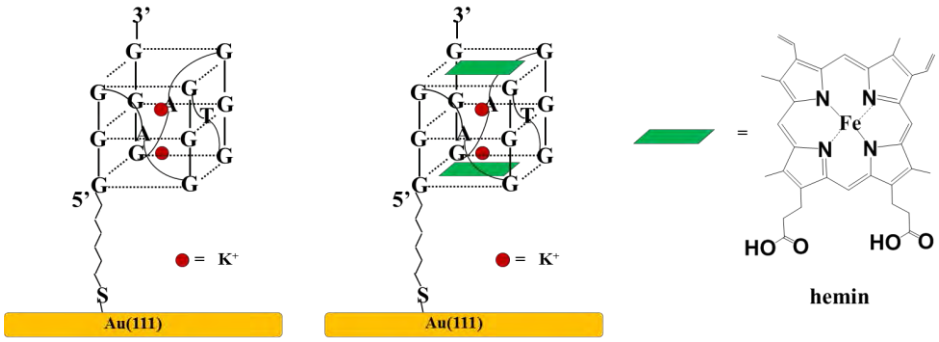

Figure 1. Schemed DNAzyme based on the G-quadruplex and hemin.

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Enzyme discovery for fucoidan modification

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Fucoidans are sulfated polysaccharides found in brown seaweeds and some marine invertebrates and they possess a variation of biological activities, including anti-cancerous. The structure of fucoidan varies substantially from a backbone of fucose linked 1-3 or 1-4, to a backbone of fucose and galactose residues, the latter called galactofucans. The detailed chemical structure of fucoidans remains largely unknown, especially fucoidans from brown seaweeds from tropical regions because of their more complicated structures (García-Ríos et al. 2012). The complicated fucoidan structure is not only caused by different sugars with several possible linkages in the backbone but also on the position of the sulfate groups on the fucose residues.

In this study, we search for fucoidanses and sulfatases able to modify fucoidans, in particular galactofucans from *Sargassum mcclurei*, a brown algae found in the Vietnamese sea. This fucoidan consists of α→3)-α-L-Fucp(2,4SO_3−)-(1→3)-α-L-Fucp(2,4-SO_3−)-(1→motif with 1,4-linked 3-sulfated α-L-Fucp inserts and 6-linked galactose in the reducing end (Thinh et al. 2013). Marine bacteria isolated from the gut of sea cucumbers are thought to produce fucoidanases and sulfatases. A new C-PAGE assay is used to identify endo-fucoidanase activity.

Initial results show that 20 different bacterial strains isolated from the sea cucumber gut are able to produce fucoidanases or sulfatases capable of modifying fucoidan from *Sargassum mcclurei*. The genomes of eight bacteria with highest fucoidan modifying activities have been identified to genus level and 11 sulfatases have been synthesized from one of the strains showing the highest level of sulfatase activity. Further work is in progress to characterize putative fucoidanases from these bacterial strains.

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Zeolite-catalyzed conversion of sucrose to fructose

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The production of fructose has lately received much industrial attention because it is a commonly used sweetener and can enter into different types of reactions leading to chemicals, such as HMF, levulinic acid, lactic acid or unsatured α hydroxy esters. Hence, it represents an important substrate for the replacement of petroleum based feedstock with renewable sources. Since fructose is an expensive product, the catalytic conversion of more common sugars, such as glucose and sucrose, represents an interesting alternative for industries. Nowadays, fructose is industrially obtained by isomerization of glucose using isomerase enzymes but enzymatic reactions present many disadvantages: they are specific and sensitive and it is not possible to gain high yields. Saravanamurugan et al. have studied the chemocatalytic isomerization of glucose to fructose and in 2013 they reported a method for the conversion of glucose in alcohol and aqueous media using zeolites. In this work, we study the possibility to convert sucrose, one of the cheapest and most abundant sugars available, into fructose. The zeolite H-USY (6) has an adequate proportion of Lewis and Brønsted acid sites for this application: by using it as catalyst, it is possible to carry out a cascade reaction (Fig. 1) that involves the hydrolysis of sucrose and the isomerization of glucose to fructose with the consequent formation of methyl glycosides in methanol. In a second step, the glycosides are hydrolyzed by water addition and high yields of fructose are obtained.

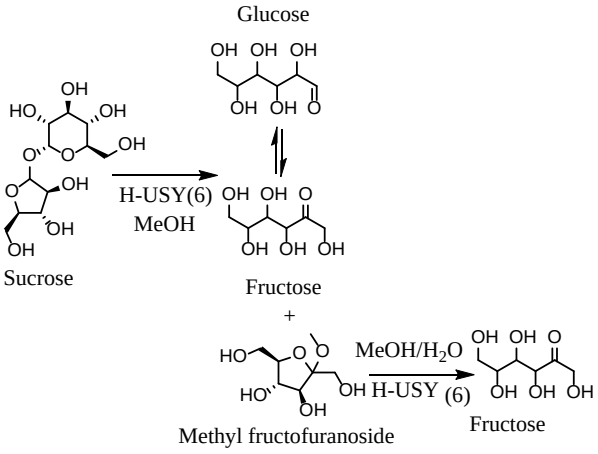

Fig. 1- Two steps hydrolysis and conversion of sucrose to fructose

The reactions were followed by 2D NMR spectroscopy. In the spectral region of primary alcohols in ^{1}H-^{13}C HSQC it is possible to distinguish the isomers of glucose, fructose and their methyl glycosides as α/β and furano/pyrano forms.[2]

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Cultivation and use of cyanobacteria for fermentation of plant biomass

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Due to the rise of the greenhouse gasses (GHGs) emission and to the intensive use of the decreasing oil resources, a high interest has developed in the area of green biotechnology focused on the production of biofuels based on renewable sources. Lignocellulosic biomass is the base for the production of second generation (2G) biofuels but its fermentation by yeast normally requires the addition of nutrients such as vitamins and minerals. This study assesses the possible exploitation of whole-cell biomass from the photosynthetic cyanobacterium *Synechococcus* sp. PCC 7002 as source of nutrients for the yeast *Saccharomyces cerevisiae* during the fermentation of low-nitrogenous lignocellulosic plant material.

A preliminary investigation of the effects of different nitrogen sources (nitrate, ammonium and urea) on the growth of *Synechococcus* was firstly performed. The cultivation of *Synechococcus* on nitrate showed that a limiting concentration caused the phenomenon of chlorosis, which is characterized by series of connected effects: bleaching of the cyanobacterial cells, degradation of the accessory light-harvesting antenna (phycobilisomes; PBS) and increase of the carbohydrate content. The tested concentrations of ammonium showed a general inhibition of growth due to a sharp acidification (pH below 5) of the growth medium which can be easily overcome by increasing the buffer capacity. In contrast, when urea was used as nitrogen source, the pH was stable but the cultures exhibited physiological nitrogen limitation effects due to the limitation of a microelement, nickel. The supply of nickel (Ni^{2+}) was required for a proper activity of urease, the metalloenzyme involved in the assimilation of urea.

Subsequently, a photo-bioreactor (PBR) was used for upscaling the production of cyanobacterial biomass grown under nitrogen-limited and non-limited conditions. The cyanobacterial biomass treated in different manners (enzymatic or acid hydrolysis) was then tested as source of nutrients for the alcoholic fermentation by the yeast on pure glucose and on the high-gravity solid feedstocks of wheat straw and spruce (dry matter content ~30 % w/w). The last-mentioned substrates previously underwent pre-treatment, enzymatic-hydrolysis and detoxification in order to render the sugar content available and to remove fermentation´s inhibitors.

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Going down subsidence lane with Sentinel-1 imagery over Denmark

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4: PPO.Labs (the Netherlands) 5: Danish Ministry of Energy, Utilities and Climate 6: NORUT (Norway)
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The Copernicus/ESA Sentinel-1 satellites' mission (S-1a & S-1b) provides the opportunity to monitor and map ongoing land surface subsidence rates with a satellite revisit time of a mere 6 days. Data are available free of charge but need collection and processing in the downstream segment to be utilized. Subsidence affects the future vulnerability to sea floods in coastal areas and tends to exacerbate climate change impact on groundwater levels and extreme precipitation, too. Besides being generally unknown if and where local Danish areas subside to an extent relevant in adaptation and mitigation, the causes and the socio-economic and environmental effects of subsidence on e.g., water management, urban planning and infrastructural design are not fully clear. Subsidence "hot spots" from modified S-1 data have been identified over three Danish cities and data over an additional 5 coastal locations are currently being analyzed to, at least, indicate potentials and use of methods in the implementation of the EU Floods Directive and in municipal climate adaptation plans in Denmark. Investigations led by the Agency for Data Supply and Efficiency will by late 2017 provide decision support for a potential operational nationwide deformation mapping using modified Copernicus/ESA Sentinel-1 imagery, Figure 1. This covers technical challenges and solutions for data processing and analysis; end-user interests, requirements and needs; business cases for selected public and commercial actors, as well as the investigations will address the setup of feedback mechanisms and communication between end-users and the scientific community (Levinsen et al., 2016; Marinkovic et al., 2016). The paper invites to join in to discuss, collaborate on and to unfold potentials of Sentinel-1 data use over Denmark.

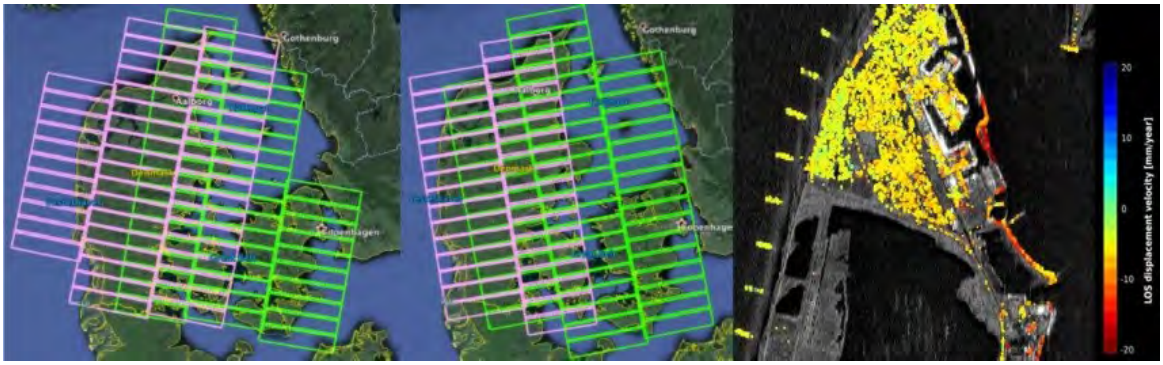

Figure 1 S-1 coverage over Denmark in ascending and descending tracks, and subsidence map over Thyborøn where orange and red colors indicate subsidence and green relative stability (right).

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Marinkovic, P., Larsen, Y., Levinsen, J.F., Broge, N., Sørensen, C. & Dehls, J. (2016). *Something is "subsiding" in the state of Denmark - Operational prospects for nationwide subsidence mapping with Sentinel-1*. ESA Living Planet Symposium 2016, Prague, Czech Republic.

Marine Climate Services - Forecasting the state of the ocean at end-user relevant time-scale

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Recent advances in oceanographic modelling mean that today we can forecast the state of the ocean with meaningful skill up to a decade in advance. Such forecasts are potentially of great value to society, as they span the gap between the short (days-to-weeks) time scales of weather forecasts and the long (century) time-scales of climate projections: importantly, these are the time-scales where most users make important decisions. However, a translation step is required to convert the outputs from these models, which are typically physical variables, into variables that are directly relevant to end-users (e.g. distribution and productivity of fish stocks) to create so-called "climate services". As an example of this process and its potential, I will describe the development of skilful forecasts of a biological variable on this 1-10 year time-scale: the distribution of bluefin tuna (*Thunnus thynnus*) in the North Atlantic. Further opportunities for forecasting variables, both globally and that are of direct relevance to Danish end-users will also be presented.

State of the Earth´s Oceans

Sigrún Huld Jónasdóttir

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The oceans cover 70% of the Earth's surface and are an essential part of the whole earth system. The oceans have a fundamental role in controlling our climate, are an important buffer for atmospheric CO_2 and are one of the most important sources of protein and lipids exploited for human consumption. In spite of their importance for climate, and exploitation our knowledge of the oceans is less than our knowledge of space.

Satellite remote sensing over last 20 years has been revolutionary for marine research as it revealed the intricate patterns of the marine environment, its currents, blooms, hot spots, upwelling zones and more. Many crucially important processes do take place at the ocean surface, such as heat flux, deep water formation, primary production. However, over and above covering the 70% of the earth's surface the Ocean is 3-Dimensional and includes over 90% of the habitable space on this planet out of the detection of satellite or other airborne sensing.

There is a need to develop observational platforms and systems that can detect processes in the deep oceans. During the last 10 years a major international effort has been on underwater ocean observation technology. Argo floats and gliders have revealed the oceans heat storage and shown that 93% of the heat associated with global warming has gone into the oceans since the industrial revolution. Undulating video plankton recorders give us information of patchiness under the ocean surfaces, green laser cameras detect organisms in murky waters of the coastal zones and new generation of sensors give us the opportunity to sniff out DNA. At DTU, we are tantalizingly close to the forefront of this innovation, innovation that is crucial for our sustainable exploitation of the world's oceans.

UTOFIA: Time-of-Flight camera for underwater applications

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Today's ever increasing proliferation of information, real-time data feeds and overwhelming sensor coverage, can often make the world feel small and constrained. However, the oceans and seas contain some of the world's most unexplored and uncharted regions, and hold valuable physical and informational resources for the planet's population. As well as the obvious mineral wealth, knowledge regarding the health and well-being of the underwater environment will become critical information over the coming years. Understanding and monitoring fish stocks, mapping the sea floor and assessing the health of the ecosystem, whilst noting the impact of human activity are becoming an increasing concern for both public and commercial bodies. UTOFIA is a H2020 project (633098) is undertaking the development, testing and commercialization of a new, compact and cost-efficient concept for underwater range-gated imaging system. It will offer a compact and cost-effective underwater imaging system for turbid environments. Using range-gated imaging, the system will extend the imaging range by factor 2 to 3 over conventional video systems. At the same time, the system will provide video-rate 3D information. This will fill the current gap between short-range, high-resolution conventional video and long-range low-resolution sonar systems. UTOFIA offers a new modus operandi for the main targeted domains of application: marine life monitoring, harbour and ocean litter detection, fisheries and aquaculture stock assessment, and seabed mapping. Progress in UTOFIA has been rapid, and we present here a summary of results from deployments of prototypes in observing marine organisms – as a demonstration of the application of the system in monitoring underwater habitats, stock assessment and for use in offshore fish farms.

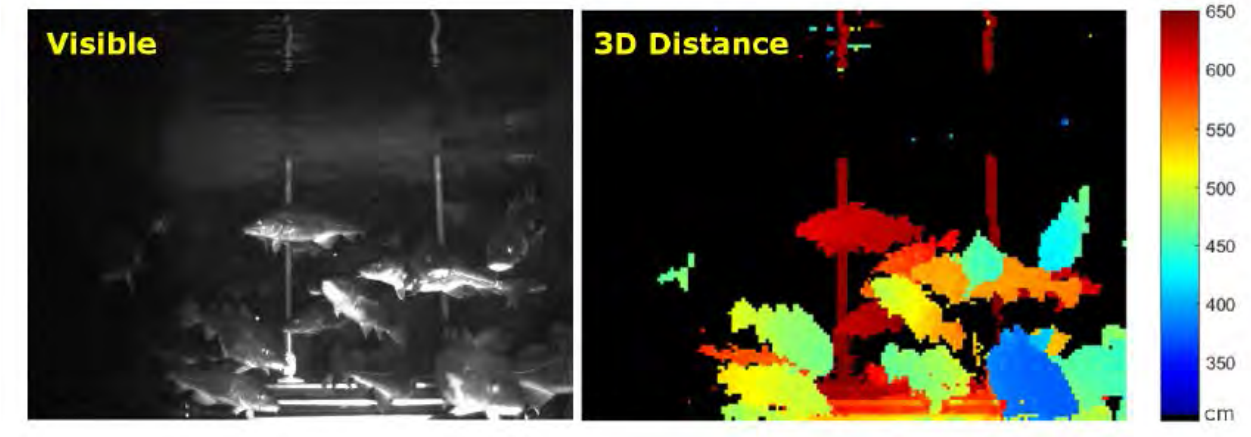

Figure: 3D reconstruction of fish swimming in a test tank from range-gated imaging.

Session

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Laptop Presentations

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Session

S

Poster Presentations

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Can the Paris Agreement stop global warming?

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At the COP21 meeting in Paris world leaders agreed to keep the Earth's temperature well below 2 degrees Celsius and preferably limit the temperature increase to 1.5 degrees Celsius above pre-industrial levels. To achieve this they decided to reduce the predicted emission of greenhouse gases in the year 2030 of about 55 Gt Carbon to 40 Gt Carbon. This can be compared to an approximate emission of 35 Gt in 2014 and thus means that a global rise in emission of only 5 Gt Carbon is allowed over the next 15 years.

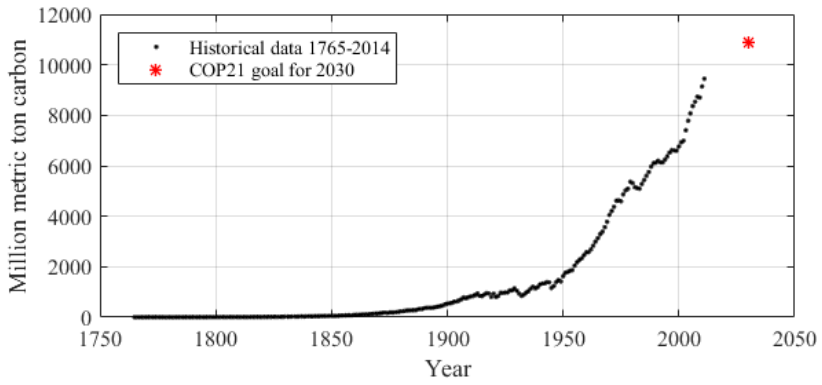

Figure 1. Historical carbon emission data and COP21 goal for 2030.

Using the Danish Center for Earth System Science (DCESS) model [1] we have investigated how large an emission reduction is necessary to keep the global temperatures below these targets.

The DCESS model is a low order Earth system box model which includes atmosphere, ocean, ocean sediment, land biosphere and lithosphere components, and using the year 1765 as the pre-industrial level.

We have examined different emission scenarios and the national commitments and find that even if the Paris Agreement is fulfilled, global temperatures will have increased by 1.5 degree C in 2030, and then only a yearly percentage reduction of 5% or more will be sufficient to keep temperatures below 2 degree C in 2100.

[1] Shaffer, G, Olsen, SM & Pedersen, JOP 2008, 'Presentation, calibration and validation of the low-order, DCESS Earth System Model'. *Geoscientific Model Development,* vol 1, no. 1, pp. 39-124. DOI: 10.5194/gmd-1-17-2008

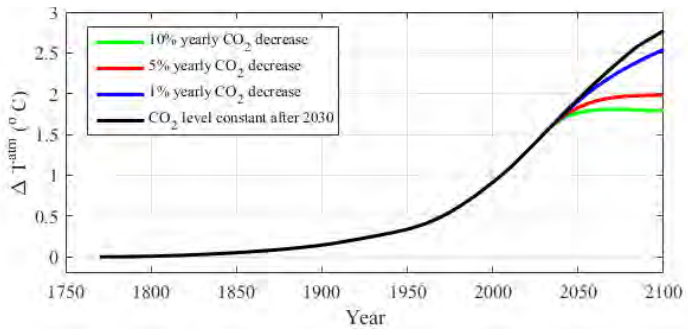

Figure 2. Temperature response to possible yearly carbon reductions.

Nex, F. and Remondino, F. (2014) 'UAV for 3D mapping applications: A review', *Applied Geomatics*, 6(1), pp. 1–15. doi: 10.1007/s12518-013-0120-x.

Shahbazi, M., Sohn, G., Théau, J. and Menard, P. (2015) 'Development and evaluation of a UAV-photogrammetry system for precise 3D environmental modeling', *Sensors (Switzerland)*, 15(11), pp. 27493–27524. doi: 10.3390/s151127493.

Singh, M. K., Gautam, R., Gatebe, C. K. and Poudyal, R. (2016) 'PolarBRDF: A general purpose Python package for visualization and quantitative analysis of multi-angular remote sensing measurements', *Computers & Geosciences*. Elsevier, 96, pp. 173–180. doi: 10.1016/j.cageo.2016.08.015.

Quantification of methane emissions from two Danish landfills

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The disposal of waste, containing organic material, in landfills results in landfill gas (LFG) generation. LFG consists of methane (55-60 %) and carbon dioxide (40-45 %). Estimates of methane emissions are required for national greenhouse gas inventories. One approach for quantification of whole landfill site emission is the tracer dispersion method. The objective of this study was to quantify methane emissions from two Danish landfills, using the tracer dispersion method.

The tracer dispersion method is based on the assumption that the landfill methane and a continuously released tracer gas (acetylene in this study) will disperse in the same way in the atmosphere. Methane emissions can be quantified by performing several traverses downwind perpendicular to the plume from the landfill while measuring the atmospheric concentration of methane and tracer gas. Gas concentrations were measured by a $C_2H_2/CH_4/H_2O$ analyzer (G2203, Picarro, Inc., Santa Clara, CA) based on Cavity Ring-Down Spectroscopy (CRDS). Two measurement campaigns were performed on January 14 and March 15, 2016. Figure 1 shows methane and tracer gas plumes measured downwind of the landfills.

Figure 1. Methane (red) and tracer gas (yellow) plumes measured downwind of the landfills. The orange triangles indicate the tracer gas release locations.

The total methane emissions from both landfills were 49.6 and 45.8 kg CH_4/h on January 14 and March 15, respectively, which equals 10,400 ton CO_2eq/year. The lower emission rate measured on March 15 in comparison to January 14 was most likely due to increasing barometric pressure on March 15. Methane emission from the composting plant was 18.9 kg/h on January 14; and was not distinguishable on March 15.

The measured methane emission rates indicate that there is a high potential for mitigation of methane emission and optimization of gas collection efficiency at the landfills. The methane oxidation and collection rates were not quantified in this study and remain a future topic to be studied. Quantification of the methane oxidation and the gas collection rate is necessary in order to calculate the gas collection efficiency and develop a plan for optimization of methane collection and mitigation of methane emission.

Session

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Oral Presentations

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Safe and Sustainable: Optimizing Material Flows in a Circular Economy

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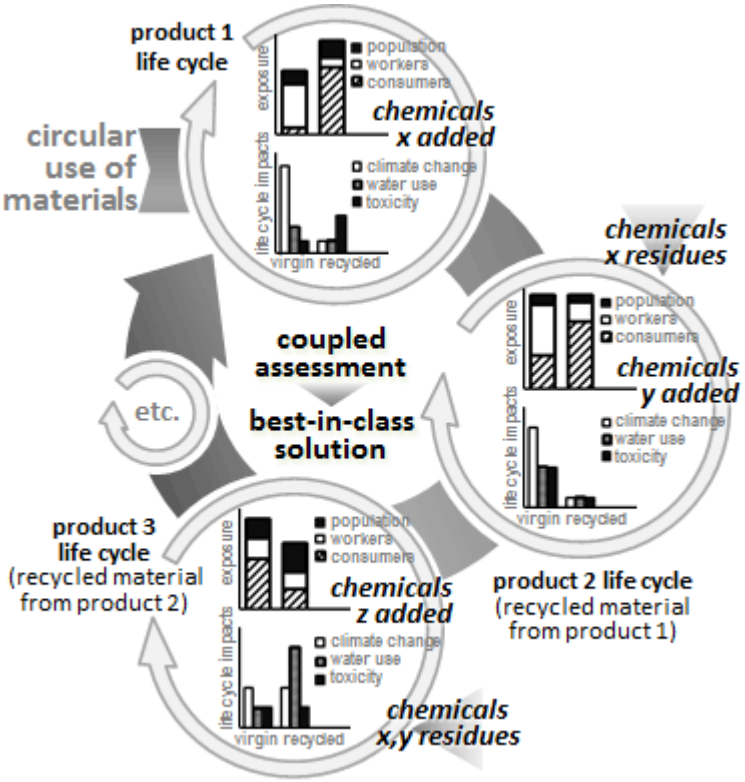
*Corresponding author email: pefan@dtu.dk

Increasing the sustainability of a globally connected economy is gaining wide attention in a world with limited natural resources and growing chemical pollution.[1] The circular economy has emerged as a way to reduce carbon and other emissions, while increasing resource efficiency over several product life cycles.[2] However, a circular economy is only viable if it is both safe and sustainable. The dilemma is that sustainable does not necessarily imply safe and vice versa. When minimizing exposure to harmful chemicals in consumer products (safe), we often use more energy-demanding alternative solutions (unsustainable). When maximizing resource use efficiency and reducing carbon and other emissions through recycling (sustainable), direct consumer exposure is often increased through cross-contamination of recycled materials (unsafe). Hence, circular economy currently fails to unite the required expertise to simultaneously increase sustainability and reduce exposure to chemicals in materials reused across life cycles of different products (see right-side Figure). For a way out of this dilemma, a paradigm shift is needed towards a comprehensive and quantitative assessment framework. In this framework, consumer, worker and population exposure is consistently coupled with life cycle impacts for materials used in consecutive product loops to identify sustainable and safe solutions for a viable, circular use of chemicals and materials.[3] This will help to achieve a safer and more sustainable circular economy through a targeted and efficient use of chemicals and materials. Based on identifying viable alternatives to harmful chemicals along material life cycles, this economy will be able to ensure controlled material recycling and successfully avoid the dilemma of safe but unsustainable or sustainable but unsafe solutions.



[1] Steffen et al. 2015. Science 347: 736-746
[2] Stahel 2016. Nature 531: 435-438
[3] Rappaport and Smith 2010. Science 330: 460-461

First order risk assessment for nanoparticle inhalation exposure based upon pulmonary inflammation and surface area dose.

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Inhalation exposure to low toxicity and biodurable particles has shown to induce polymorphonuclear neutrophilia (PMN) in the lungs, which is a strong indicator for lung inflammation. Schmid and Stoeger (2016) revised mice and rat intratracheal instillation studies and assessed the relation between particles dry powder BET surface area dose and PMN influx for granular biodurable particles (GBPs) and transition metal oxides. Koivisto *et al.* measured workers alveolar lung deposited surface area (LDSA) concentrations ($\mu m^2\ cm^{-3}$) during injection molding of polypropylene (PP) car bumpers (Figure 1a) and production of tungsten-carbide-cobalt (WCCo) fine grade powder using diffusion chargers. First order risk assessment was performed by comparing the doses calculated from measured LDSA concentrations during an 8-h work day with the $NOEL_{1/100}$, the one hundredth of no observed effect level, assigned for GBPs (0.11 $cm^2\ g^{-1}$; Figure 1b) and transition metal oxide particles ($9\times10^{-3}\ cm^2\ g^{-1}$). During the injection molding of PP car bumpers, LDSA concentrations varied from 23 to 39.8 $\mu m^2\ cm^{-3}$ corresponding 8-h dose at a maximum of $1.4\times10^{-3}\ cm^2\ g^{-1}$.

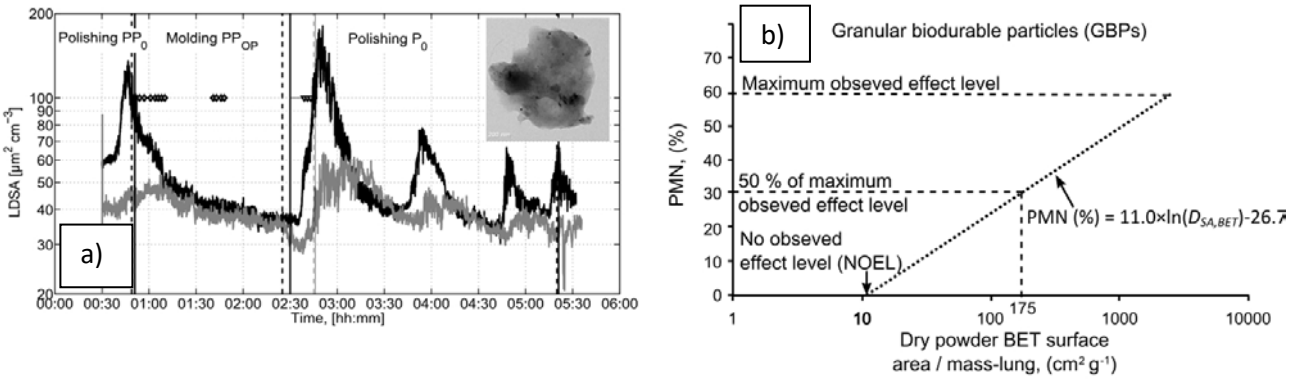

Figure 1. a) LDSA concentrations during PP injection molding and PMN-dose-response as BET surface area.

Schmid O, Stoeger T, 2016. Surface area is the biologically most effective dose metric for acute nanoparticle toxicity in the lung. *J. Aerosol. Sci.* 99, 133-143.

Koivisto AJ, Kling KI, Levin M, Fransman W, Gosens I, Cassee FR, Jensen KA. First order risk assessment for inhalation exposure during injection molding of polypropylene composites and production of tungsten-carbide-cobalt fine powder based upon pulmonary inflammation and surface area dose. In review at *NanoImpact*.

Automated Scanning Electron Microscopy Analysis of Sampled Aerosol

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Airborne fine and ultrafine particles (aerodynamic diameters less than 2.5 and 0.1 µm respectively) have in recent years been recognized as major concerns for public health, due to their ability to penetrate deep into the lungs or even into the blood stream. Recent studies have furthermore found that parameters such as morphology, size, number concentration, surface area, as well as the chemical composition of particles have a high influence on the observed toxicological effects. However current aerosol legislations focus only on aerosol mass, meaning that small particles are poorly regulated due to their small contribution to the total aerosol mass concentration. New or additional legislations and measurement techniques are therefore needed to deal with the complexity of aerosols in order to establish standard procedures for measuring and regulating aerosol exposure.

Here we present the current development of an automated software-based analysis of aerosols using Scanning Electron Microscopy (SEM) and Scanning Transmission Electron Microscopy (STEM) coupled with Energy-Dispersive X-ray Spectroscopy (EDS). The automated analysis will be capable of providing both detailed physical and chemical single particle information not provided by the current standard methods. Physical parameters such as area, diameter, aspect ratio, aggregation state, and estimates of surface area will be obtained for each individual particle based on the acquired images, while automated EDS analysis will yield single particle elemental composition data, allowing size resolved chemical classification of each individual particle. The automated analysis will furthermore be able to systematically map large areas of a sample without user intervention, enabling a fast and repeatable measurement, while obtaining sufficient data for statistical analysis.

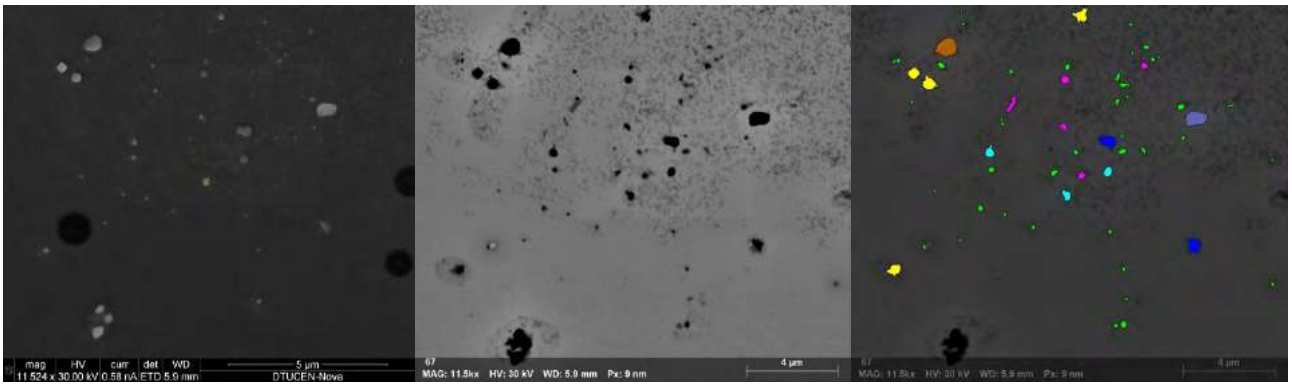

Figure 1. SEM images obtained from the automated analysis of an aerosol sample. Left: secondary electron (SE) image; Middle: Corresponding STEM image, which is used for sizing and particle recognition; Right: STEM image where the automated program has marked the recognized particles, which will automatically be analyzed further both with sizing tools and EDS to yield their elemental composition.

Exposure characterization of nanoparticles in different workplace environments

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Exposure to nanoscale particles (particle diameter < 100 nm) has been widely linked to adverse health effects and is considered one of the major current emerging risks in workplaces [1]. In the workplace, workers may be exposed to nanoscale particles while dealing with engineered nanoparticles (ENP) or process-generated nanoparticles (PGNP) during industrial processes involving unintentional nanoparticle release or the formation of nanoparticles from gaseous precursors [2, 3, 4]. Due to the relative novelty of "nanosafety" as a field of research, relevant studies about ENP and PGNP release and exposure under real-world conditions are scarce.

This work investigates different nanoparticle exposure scenarios, dealing with both ENP (exposure scenarios #1 to #3; Figure 1) and PGNP from ceramic processes (exposure scenarios #4 to #10; Figure 1). In addition to emissions and potential particle transformations in workplace air, the potential for particle release to the outdoor environment, and the effectiveness of control measures were also assessed. A multi-instrument approach was used to characterise source-specific worker exposure, aiming to cover the most relevant nanoparticle metrics and physicochemical properties. Overall, nano-sized particles were generated and emitted into workplace air on a statistically significant level [5] and above the available nano-reference values (NRV; 4 x 10^4 cm^{-3}) during all of the processes evaluated (with the exception of single walled carbon nanotubes manufacturing; exposure scenarios #1 to #2). The effectiveness of the mitigation measures in place in the environments assessed were tested and results showed that the use of appropriate strategies may reduce worker exposure to nanoparticles by up to 98%.

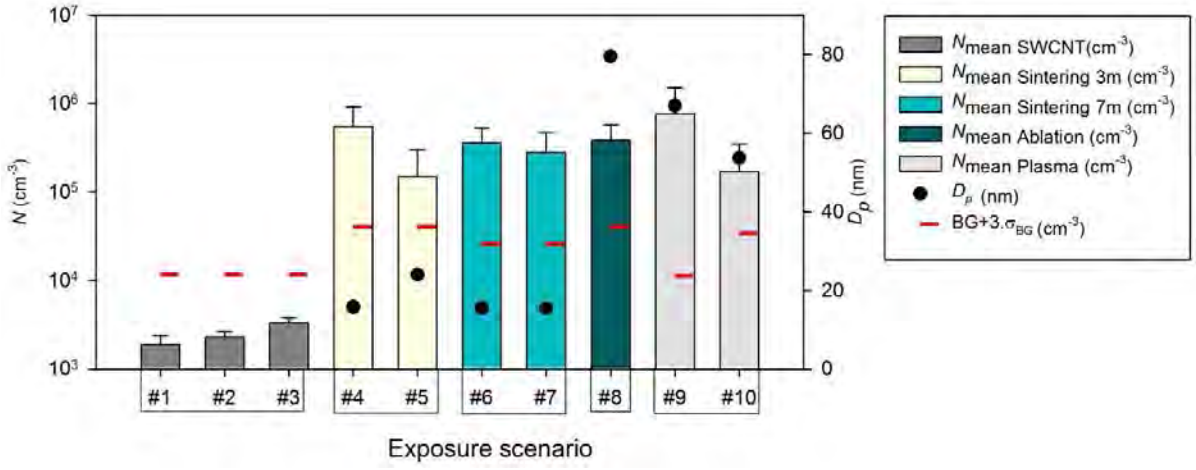

Figure 1. Particle number concentrations and mean particle diameter measured in the breathing zone for each of the exposure scenarios analysed, as well as the significance level of particle exposure during each activity (BG+3.σ_{BG}).

References

[1] EU-OSHA (2009) Workplace Exposure to Nanomaterials. European Agency for Safety and Health at Work.
[2] Koivisto *et al*. (2014) *Int. J. Environ. Res. Public Health.* 11: 5382-5402.
[3] Fonseca *et al*. (2016) *Science of The Total Environment.* 565: 922–932.
[4] Fonseca *et al*. (2016) *Ann Occup Hyg. 59*:586-599.
[5] Asbach et al. (2012) *NanoGEM.* SOP for assessing exposure to nanomaterials, following a tiered approach.

Session

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Laptop Presentations

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Non-plastic food contact materials: classification of chemicals using predictive models

Elena Boriani[1,2], Eelco Pieke[2], Eva Wedebye[2], Emilio Benfenati[3], Kit Granby[2], Tine Hald[2]

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A recently report on the implementation of the Food Contact Materials Regulations ((EC)No 1935/2004)[i] states that there is insufficient information on human exposure to chemicals from Food Contact Materials (FCMs) to consider their safety. In particular, the EU legislation is still lacking information for many compounds that can be found in non-plastic FCM (e.g. recycled paper and board).[ii] While recycled materials may support circular economy, the same materials may pose a risk to humans, if potentially harmful compounds that are able to migrate from the packaging material to the food, are not avoided.

The work we are conducting on non-plastic FCMs aims to develop models that are able to predict the harmful effects of chemical compounds possibly present in FCMs, thereby providing a tool for further prioritization.

We used a library of around 4500 compounds extracted from databases at EFSA[iii], UK Health Ministry, FDA[iv], JRC[vvi], NIAS[vii], as well as in-house data derived from two PhD theses[viii,ix]. The main objective is to provide information to close the identified data gaps regarding human exposure to non-plastic FCMs.

We present the results obtained so far using different software and databases with the aim of classifying compounds. We started predicting carcinogenicity, developmental toxicity and mutagenicity properties of the library compounds using VEGA[x], the Danish QSAR database and Toxtree models[xi]. In addition, the work is performed in parallel with experimental work at DTU Food to identify possible new chemicals present in different non-plastic FCM packaging items.

The combination of these works is preparatory for a comprehensive decision support analysis that will also assess the environmental impact of non-plastic FMCs.

[i] ENVI Committee (July 18, 2016). "Report on the implementation of the Food Contact Materials Regulation ((EC) No 1935/2004)." European Parliament
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Session

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Poster Presentations

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Direct vacuum inlet system enabling highly sensitive in-situ analysis of chemical reaction products

Daniel B. Trimarco, Søren B. Scott, Thomas Pedersen, Ole Hansen, Ib Chorkendorff and Peter C. K. Vesborg

Electrochemical reactions play an increasingly important role in sustainable energy conversion and chemical synthesis. Better understanding of catalytic mechanisms at electrode surfaces is thus important for the transition to a clean-energy economy, but is hindered by the difficulty of real-time detection of products and reaction intermediates during electrochemistry experiments. Electrochemical mass spectrometry (EC-MS), including techniques referred to as DEMS and OLEMS, can enable in-situ detection of electrochemical products, but often fails to provide quantitative or reproducible results.

Herein, we present a new type of EC-MS based on a versatile gas inlet to vacuum fabricated onto a silicon microchip, and compare it to established techniques with focus on sensitivity, time response, and mass transport. The chip consists of a perforated membrane stablizing a large liquid-gas interface, a capillary maintaining a controlled flow over a pressure drop to ultra-high vacuum, and inlet and outlet channels for an inert make up gas. The use of a direct inlet enables orders of magnitude higher sensitivity than differentially pumped systems without a loss in time response for volatile products, while clean-room techniques for chip fabrication and a precicely controlled working distance between the electrode and chip membrane provide for a highly reproducible experimental setup. The make up gas can also be used to saturate the electrolyte from through the chip membrane enabling quick and precise exchange of dissolved gases. The well-characterized mass transport of both reactants and products in this setup enables single-turnover resolution for analysis of electrochemical reactions, as will be demonstrated with examples.

Development of a QSAR Model for Thyroperoxidase Inhibition and Screening of 72,526 REACH substances

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Thyroid hormones (THs) are involved in multiple biological processes and are critical modulators of fetal development. Even moderate changes in maternal or fetal TH levels can produce irreversible neurological deficits in children, such as lower IQ. The enzyme thyroperoxidase (TPO) plays a key role in the synthesis of THs, and inhibition of TPO by xenobiotics results in decreased TH synthesis. Recently, a high-throughput screening assay for TPO inhibition (AUR-TPO) was developed and used to test the ToxCast Phase I and II chemicals. In the present study, we used the results from AUR-TPO to develop a Quantitative Structure-Activity Relationship (QSAR) model for TPO inhibition. The training set consisted of 898 discrete organic chemicals: 134 inhibitors and 764 non-inhibitors. A five times two-fold cross-validation of the model was performed, yielding a balanced accuracy of 78.7%. More recently, an additional ~800 chemicals were tested in the AUR-TPO assay. These data were used for a blinded external validation of the QSAR model, demonstrating a balanced accuracy of 85.7%. Overall, the cross- and external validation indicate a robust model with high predictive performance. Next, we used the QSAR model to predict 72,526 REACH pre-registered substances. The model could predict 49.5% (35,925) of the substances in its applicability domain and of these, 8,863 (24.7%) were predicted to be TPO inhibitors. Predictions from this screening can be used in a tiered approach to prioritize potential thyroid disrupting chemical substances for further evaluation. *This abstract does not necessarily reflect U.S. EPA policy*

Circular and Safe?

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The European Commission's action plan prepares the move towards a circular economy to reduce waste and to reuse more efficiently the value of products and resources. Increased recycling of packaging materials is part of this plan, and the Commission has set an ambitious goal of 55 % of plastic packaging recirculation in 2025. This puts a pressure on increased reuse of plastic materials in food packaging which represents a large application of plastics in Europe.

However, recirculation and reuse in food packaging materials introduces serious challenges to the safety. Many studies on recirculated paper and board have shown that such materials are often contaminated with chemicals from their previous use and represent a potential significant source of human exposure to many chemicals, including CRM substances. In spite of the scientific knowledge from an extensive amount of analytical work in this field and use of many resources in risk evaluations over the last decade this problem has not been managed successfully, indicating the challenges that lie ahead if the use of recycled materials in food packaging is extended to plastic materials. Indeed, recent studies have already reported on chemicals of concern found in recirculated plastics

In the Commission's action plan the demand for increased recirculation is primarily justified by expected economic and environmental benefits. This also seems to be the focus point for the expressed need for quality standards for the secondary raw materials. In order to keep control of the future potential exposure of humans to chemicals in food packaging plastics, quality standards have to be implemented already for the primary raw materials in a circular economy since it will be challenging to keep track of individual materials recirculated in different products through consecutive recycling loops. The standards must apply for all plastics with a potential to end up in food packaging after recycling and address the use of chemicals and in particular their safety towards human health. Regulation according to such standards is a daunting task, but if it is neglected, chemicals of concern can become a severe barrier to achieve high quality and safe materials produced from secondary raw materials and then the circular economy can ruin the current achievement of plastic food packaging materials being a well regulated area in EU.

Possible implications and solutions in the food packaging area will be discussed.

Session

W

Oral Presentations

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Session

W

Laptop Presentations

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What does it take to practice sustainable flood risk management?

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Flood risk is often handled through flood risk management frameworks; here the risk is quantified and translated into a societal cost. Then, alternative scenarios are defined as solutions and they are ranked according to both the cost of expected damage and the cost making changes to the system. Merz et al. (2014) summarize challenges in flood risk management that illustrate how flood risk management already require assessment of sustainability aspects today, although sometimes unconsciously. Environmental sustainability is often assessed using life cycle assessment (LCA), but this is still rarely the case for sustainable urban water management (Belmeziti et al., 2015). Based on the flood risk decision framework proposed by Åström et al. (2014), possible options in the decision making where sustainability can be assessed are identified. This framework aims at stabilizing the flood risk over the technical lifetime of the system under study and ensures equity in an inter-generational light by spreading out investments. The environmental sustainability has to be quantified in order to be integrated in the decision framework (e.g. through LCA as in Brudler et al. (2016)). Environmental sustainability can be explicitly assessed at three stages in the decision process given that a certain risk level is to be met: 1) when formulating possible adaptation scenarios, 2) as an overall, but separate, constraint on the utility function used in the optimization at the same level as the economical constraint, or 3) through monetization along with the other consequences assessed adding to the economical constraint. This leads to decisions that follow:

- In case of small economic differences between scenarios, the most sustainable solution is chosen.
- In case of small differences in environmental impacts among scenarios, the most economical beneficial solution is chosen.
- In case of large variation between scenarios (regarding both economic and environmental impact), an assessment can be made to secure a solution that is most societal beneficial with respect to both safety and sustainability.

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Pyrolysis of sewage sludge and the issue of drying

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In the process of treating waste water, Pyrolysis has shown to be not only of economical value, but also to reduce pollutants associated with sludge[1]. Although there are fractionally more efficient technologies available in terms of maximizing the energy extraction from the sludge, none are comparable to low temperature pyrolysis when it comes to the low capital cost for manufacture and installation. Unlike other approaches such as gasification or digestion where the energy content from the sludge is aimed to be captured in the biogas, pyrolysis produces a bio-oil. This can have numerous practical advantages, particularly if the fuel is not to be used at the sewage plant but transported elsewhere. With its low sulfur characteristics the oil has also reported to have a premium application for shipping fuel.

Pyrolysis can also be uses effectively as a secondary process after digestion. It is common misconception that digested sludge does not have enough energy to warrant pyrolysis, in our experiments it has been shown that there is still enough energy left and is in line the 1/3rd energy reduction reported in[1]. The oil produced from the pyrolysis of digested sludge is plenty to support a business model, with equipment payback in less than 6 months. However, this is far from the only benefit, since the pyrolysis process leads to a dramatic reduction in waste material, which is costly to dispose of. By after the pyrolysis of a typical dewatered digested sludge the waste content to be disposed of is reduced to around just 10% by mass while the phosphor content remains, making it suitable for agriculture.

The major issue that remains is the drying process. Pyrolysis requires that the sludge be dried to 9% water content at maximum. In warmer climates it is possible to use solar drying beds. In northern climates, fueling drying ovens is required and somewhat undermines the economy of the whole process. Several approaches have been proposed to combat this issue, including microwave heating[2] and impulse drying[3], however, none have prevailed and the trend is to move away from the use of drying ovens or using the fuel produced to run the ovens.

In order to achieve a more sustainable solution, we must turn to district heating to provide low-grade heat from sludge drying. This may come from excess process heat and flue gas from the waste water treatment process or from neighboring process industries.

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Session

W

Poster Presentations

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Innovative microbial electrochemical process for H_2O_2 synthesis and residual H_2O_2 removal for wastewater treatment

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Sustainable H_2O_2 synthesis and residual H_2O_2 removal are key challenges to the treatment of recalcitrant wastewater using Fenton processes. In this study, an innovative bioelectrochemical system was developed to meet the challenges by alternate switching between microbial electrolysis cell (MEC) and microbial fuel cell (MFC) mode of operation. In the MEC mode, H_2O_2 was produced and then reacted with Fenton's reagent (Fe II) to form hydroxyradical. When the system was switched to MFC mode, the unused H_2O_2 as residual is removed at the cathode as electron acceptor. For wastewater containing 50 mg L^{-1} methylene blue (MB), complete decolorization and mineralization was achieved in the MEC mode with apparent first order rate constants of 0.43 and 0.22 h^{-1}, respectively. After switching the system to the MFC mode, unused H_2O_2 at concentration of 180 mg L^{-1} was removed. The removal rate was 4.61 mg L^{-1} h^{-1} while maximum current density of 0.49 A m^{-2} was generated. The MB degradation and removal of unused H_2O_2 were affected by different operational parameters such as external resistance, cathode pH and initial MB concentration. Furthermore, stack operation greatly improved the system performance. This study for the first time demonstrated an efficient and cost-effective bioelectrochemical system for H_2O_2 generation, residual removal and treatment of recalcitrant pollutants.

Zhang Y. , Wang Y., Angelidaki I. (2015) Alternate switching between microbial fuel cell and microbial electrolysis cell operation as a new method to control H_2O_2 level in Bioelectro-Fenton system. Journal of Power Sources, 291: 108-116

Session

X

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Intelligent water metering for private households

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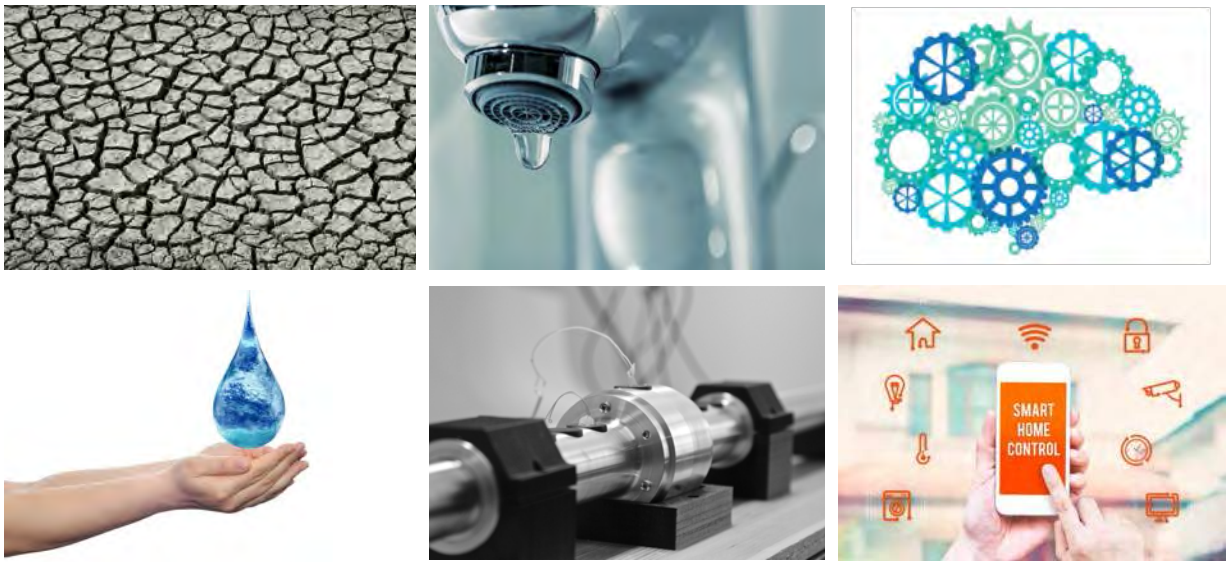

Clean water is becoming an ever more limited resource in developed and developing countries alike. To prevent critical water scarcity, we need to save water on a global scale.

Increased consumption awareness is an easy way to water savings. By identifying leaks and misuse, increased awareness can inspire people to reduce their water consumption by approximately 15 percent.

Based on a novel flow measurement technology from DTU [1], Aqubiq is developing an intelligent water metering solution for private households, enabling leak detection and water savings for private consumers. The key to this lies in big data analytics. Our principle is *more data for less water*.

In addition, Aqubiq promises to donate an equivalent 15 percent of the profit to clean water initiatives on a global scale. In that way, water savings in Denmark can help bring water to regions short on water.

In this poster presentation, we introduce the principles behind the intelligent water metering solution and demonstrate it with an early prototype.

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DTU Fundraisers stand:
Assisting you on competitive Horizon2020 proposals

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When you have decided to apply for funding from Horizon2020, it's not always easy to navigate around the participant portal. Where to find relevant calls? How does it work? Am I eligible to apply? How to set up the application? What about collaborators? Any tips and tricks?

We at DTU research support will help you with the application – from the early counselling to the final submission of a competitive proposal.

Our research support unit is a new set-up centrally at DTU where we take advantage of the synergy from bringing together each of our individual experience from decades of research support.

What we can offer you – examples:

- Counselling (finding relevant calls, interpretation of call text, planning the process)
- Commenting on the draft application
- Tools for communication, exploitation, management, impact etc.
- Participant portal (forms and formalities, including letters of support and documentation)
- Workshops (information meetings, workshops, master classes)

You can find our contacts here:
http://portalen.dtu.dk/DTU_Generelt/APK/Forskningskontoret/ekstern_finansiering.aspx